LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM093024\
Data File : BM047722.D
Acq On : 30 Sep 2024 18:34
Operator : RC/JU
Sample : P4018-16
Misc :
ALS Vial : 12 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: BM047722.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	53	rVB	39330	55377	0.17%	0.062%
2	3.675	114	117	128	rBV	231943	359155	1.08%	0.399%
3	4.928	324	330	339	rBV	470580	642503	1.93%	0.715%
4	6.134	527	535	542	rBV	609937	884679	2.66%	0.984%
5	6.975	671	678	689	rBV	654894	1029734	3.10%	1.145%
6	7.140	700	706	720	rVB	524842	824992	2.48%	0.917%
7	7.346	734	741	751	rBV	621748	984636	2.96%	1.095%
8	7.445	753	758	767	rVB2	34413	57639	0.17%	0.064%
9	7.810	812	820	828	rBV	852430	1349896	4.06%	1.501%
10	8.051	855	861	867	rVB	141220	218497	0.66%	0.243%
11	8.516	932	940	950	rBV	807423	1297875	3.90%	1.443%
12	8.963	1006	1016	1026	rBV	609007	1014452	3.05%	1.128%
13	9.534	1106	1113	1119	rBV2	65774	105517	0.32%	0.117%
14	9.687	1131	1139	1147	rBV	469057	789532	2.37%	0.878%
15	9.763	1147	1152	1157	rVV	32164	58163	0.17%	0.065%
16	9.845	1161	1166	1171	rVV3	26326	44739	0.13%	0.050%
17	9.904	1171	1176	1182	rVB3	22015	38619	0.12%	0.043%
18	10.104	1203	1210	1220	rVB	44751	82460	0.25%	0.092%
19	10.222	1223	1230	1238	rBV	786150	1320509	3.97%	1.469%
20	10.486	1268	1275	1286	rVB	142827	241328	0.73%	0.268%
21	10.604	1286	1295	1304	rBV	1164222	1966918	5.91%	2.187%
22	10.734	1308	1317	1325	rBV	743547	1302731	3.92%	1.449%
23	10.804	1326	1329	1335	rVB2	28553	49094	0.15%	0.055%
24	10.898	1340	1345	1351	rVB	38172	65811	0.20%	0.073%
25	11.139	1379	1386	1393	rVB5	25520	48360	0.15%	0.054%
26	12.028	1531	1537	1542	rBV4	21641	44271	0.13%	0.049%
27	12.128	1548	1554	1561	rBV	54710	94475	0.28%	0.105%
28	12.692	1644	1650	1658	rBV4	23070	46787	0.14%	0.052%
29	13.851	1841	1847	1854	rVB	1503251	2043179	6.14%	2.272%
30	14.080	1879	1886	1889	rBV6	18413	34297	0.10%	0.038%
31	14.139	1889	1896	1903	rVB	1670867	2504707	7.53%	2.785%
32	14.357	1927	1933	1940	rBV	2379795	3104769	9.33%	3.453%
33	14.445	1940	1948	1955	rBV	1726225	2493492	7.50%	2.773%
34	14.592	1969	1973	1975	rBV	85968	105793	0.32%	0.118%
35	14.633	1975	1980	1994	rVB	618097	931334	2.80%	1.036%
36	14.757	1996	2001	2006	rBV	84466	138327	0.42%	0.154%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM093024\
Data File : BM047722.D
Acq On : 30 Sep 2024 18:34
Operator : RC/JU
Sample : P4018-16
Misc :
ALS Vial : 12 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	14.810	2007	2010	2015	rVB3	29764	40186	0.12%	0.045%
38	14.898	2021	2025	2032	rBV5	19865	41227	0.12%	0.046%
39	14.986	2032	2040	2049	rBV3	91160	230466	0.69%	0.256%
40	15.069	2049	2054	2062	rVB	567644	849351	2.55%	0.945%
41	15.204	2073	2077	2085	rVV2	86181	136483	0.41%	0.152%
42	15.280	2085	2090	2100	rVB3	106220	207432	0.62%	0.231%
43	15.433	2107	2116	2124	rBV	2224602	3174176	9.54%	3.530%
44	15.545	2129	2135	2150	rBV2	657142	1068397	3.21%	1.188%
45	15.680	2153	2158	2161	rBV4	25733	47690	0.14%	0.053%
46	15.798	2172	2178	2183	rBV	749117	1021535	3.07%	1.136%
47	15.851	2183	2187	2193	rVB4	47339	73344	0.22%	0.082%
48	16.074	2219	2225	2229	rBV5	31922	58829	0.18%	0.065%
49	16.163	2236	2240	2243	rBV	46787	60152	0.18%	0.067%
50	16.263	2252	2257	2263	rVB3	47119	70937	0.21%	0.079%
51	16.363	2268	2274	2279	rBV7	39798	85661	0.26%	0.095%
52	16.510	2293	2299	2305	rBV8	36867	71605	0.22%	0.080%
53	16.568	2305	2309	2316	rVB6	24506	41620	0.13%	0.046%
54	16.745	2335	2339	2345	rVB8	16251	34322	0.10%	0.038%
55	16.845	2345	2356	2370	rBV	19850226	33260377	100.00%	36.989%
56	16.951	2371	2374	2378	rVV2	83614	138233	0.42%	0.154%
57	16.998	2378	2382	2390	rVB6	57168	118086	0.36%	0.131%
58	17.186	2407	2414	2421	rBV	2100960	3040847	9.14%	3.382%
59	17.280	2424	2430	2436	rVV	2457328	3404621	10.24%	3.786%
60	17.327	2436	2438	2447	rVB3	90006	114077	0.34%	0.127%
61	17.474	2458	2463	2470	rBV7	61782	122394	0.37%	0.136%
62	17.545	2470	2475	2478	rVV5	31562	57695	0.17%	0.064%
63	17.574	2478	2480	2488	rVB7	31947	56798	0.17%	0.063%
64	17.686	2495	2499	2502	rBV2	36559	47272	0.14%	0.053%
65	17.762	2507	2512	2515	rVV	117356	163169	0.49%	0.181%
66	17.798	2515	2518	2525	rVB3	115617	154607	0.46%	0.172%
67	18.074	2560	2565	2573	rBV	305721	445411	1.34%	0.495%
68	18.380	2614	2617	2626	rVB6	33701	66732	0.20%	0.074%
69	18.462	2627	2631	2635	rVV4	30198	38153	0.11%	0.042%
70	19.004	2721	2723	2731	rVB8	31675	57001	0.17%	0.063%
71	19.133	2741	2745	2752	rVB3	31573	48135	0.14%	0.054%
72	19.204	2753	2757	2761	rBV2	31876	45827	0.14%	0.051%
73	19.351	2778	2782	2786	rBV4	71402	100853	0.30%	0.112%
74	19.562	2812	2818	2826	rBV	2903638	3982725	11.97%	4.429%
75	21.080	3072	3076	3082	rBV3	199989	303518	0.91%	0.338%
76	21.403	3125	3131	3139	rBV	2091733	3062863	9.21%	3.406%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM093024\
Data File : BM047722.D
Acq On : 30 Sep 2024 18:34
Operator : RC/JU
Sample : P4018-16
Misc :
ALS Vial : 12 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	24.203	3598	3607	3618	rBV	1606515	3898775	11.72%	4.336%
78	24.409	3633	3642	3657	rVB	1342947	3504293	10.54%	3.897%

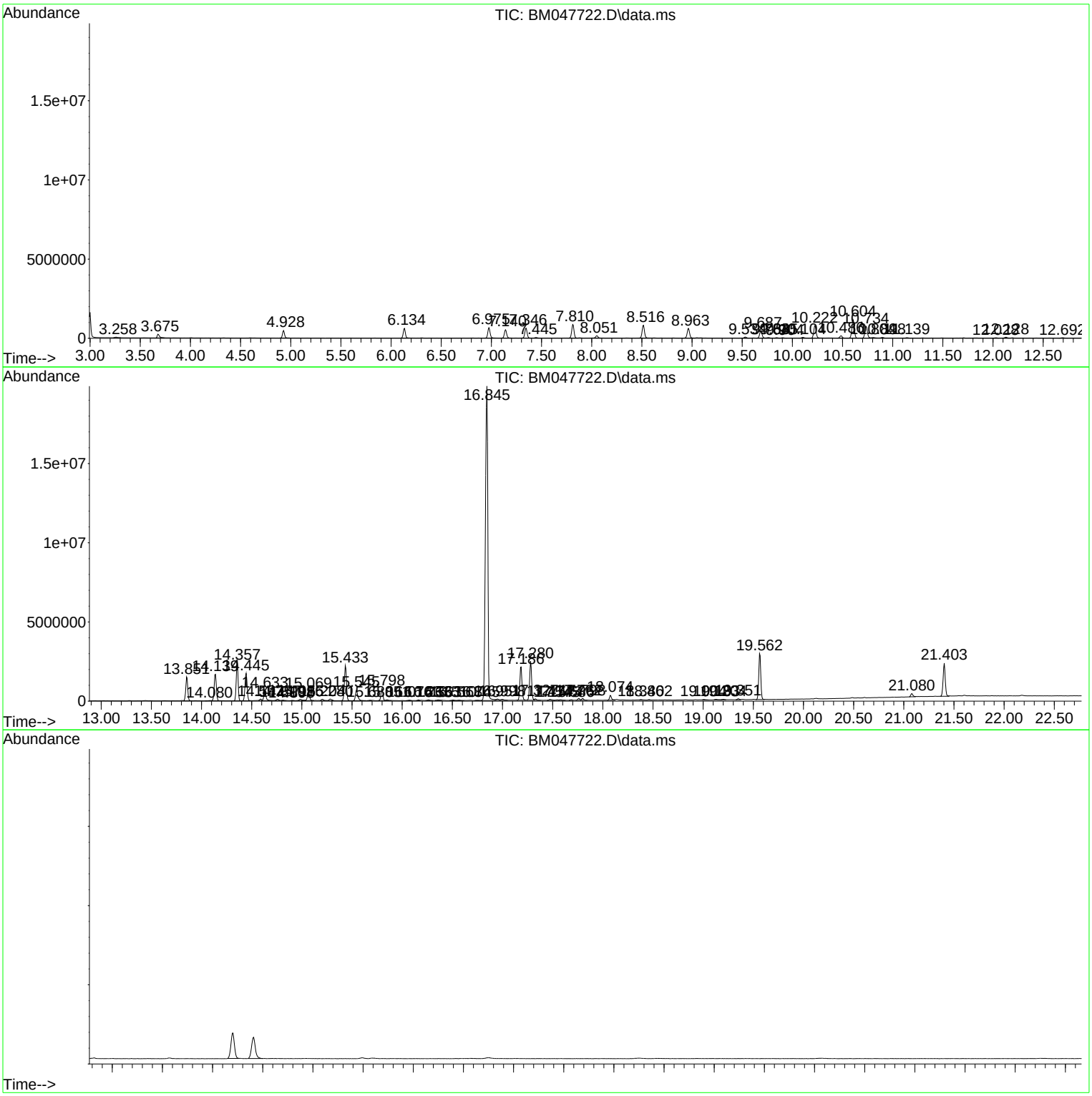
Sum of corrected areas: 89920522

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM093024\
Data File : BM047722.D
Acq On : 30 Sep 2024 18:34
Operator : RC/JU
Sample : P4018-16
Misc :
ALS Vial : 12 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\BM093024\
Data File : BM047722.D
Acq On : 30 Sep 2024 18:34
Operator : RC/JU
Sample : P4018-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DDCE2

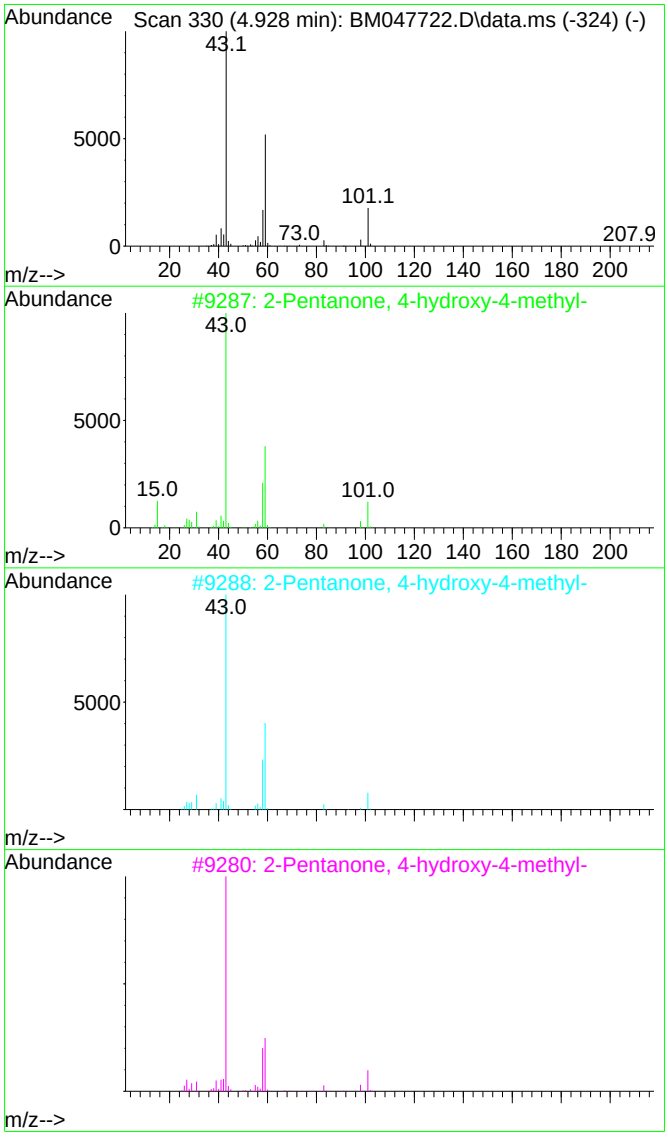
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM092724.MA.M
Quant Title : SVOA CALIBRATION

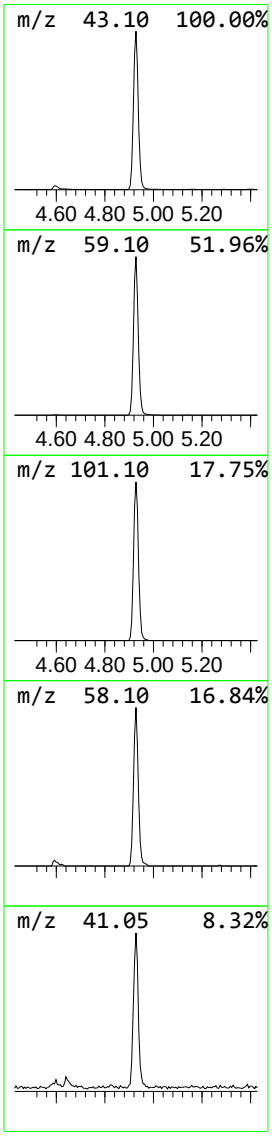
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.928	9.52 ng/ul	642503	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	45
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
4	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
5	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM093024\
Data File : BM047722.D
Acq On : 30 Sep 2024 18:34
Operator : RC/JU
Sample : P4018-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DDCE2

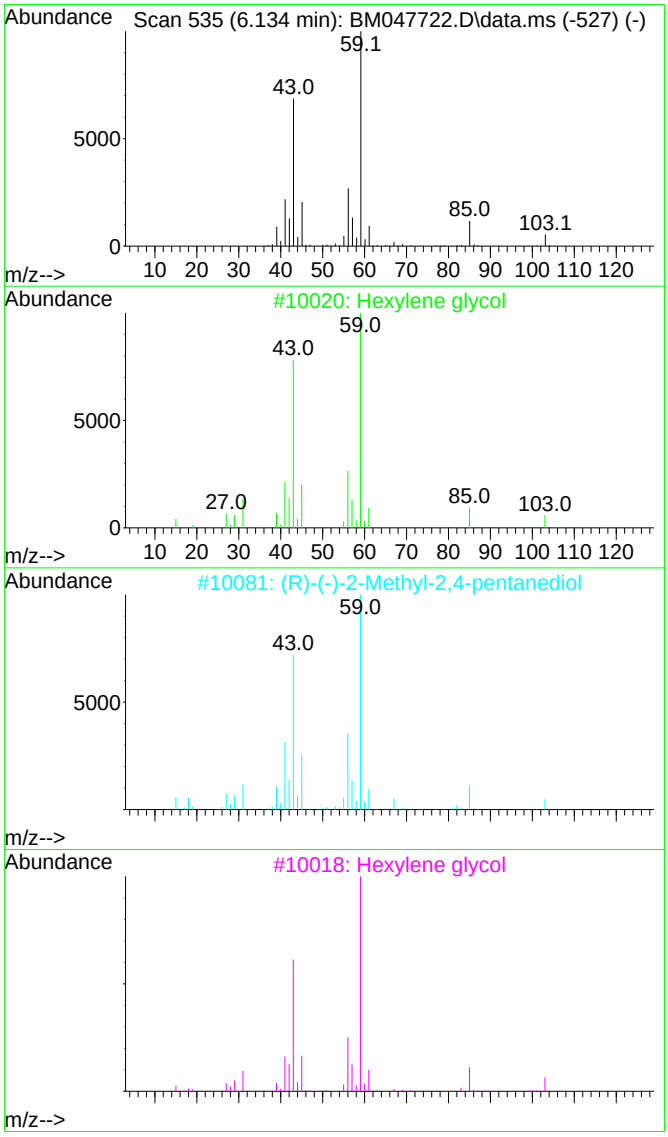
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM092724.MA.M
Quant Title : SVOA CALIBRATION

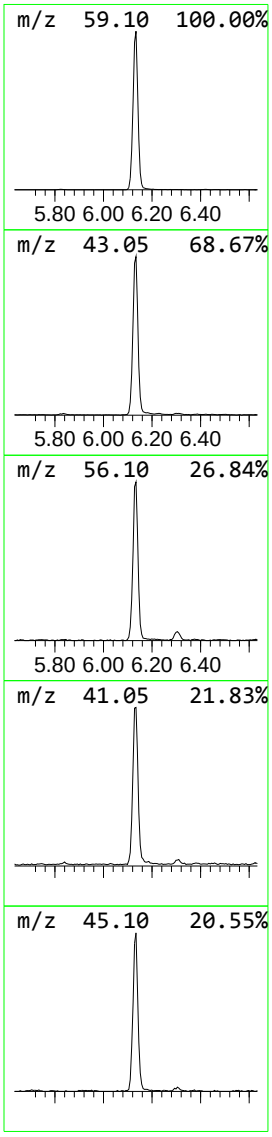
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Hexylene glycol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.134	13.11 ng/ul	884679	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	90
3	Hexylene glycol	118	C6H14O2	000107-41-5	90
4	Hexylene glycol	118	C6H14O2	000107-41-5	59
5	Hexylene glycol	118	C6H14O2	000107-41-5	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM093024\
Data File : BM047722.D
Acq On : 30 Sep 2024 18:34
Operator : RC/JU
Sample : P4018-16
Misc :
ALS Vial : 12 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

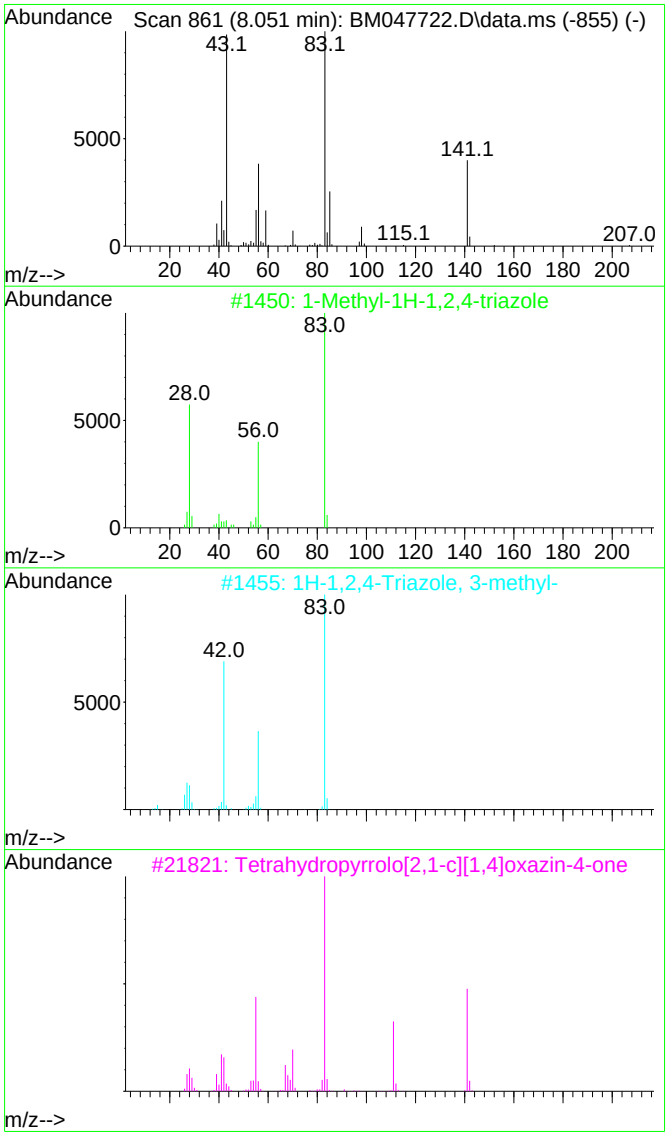
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

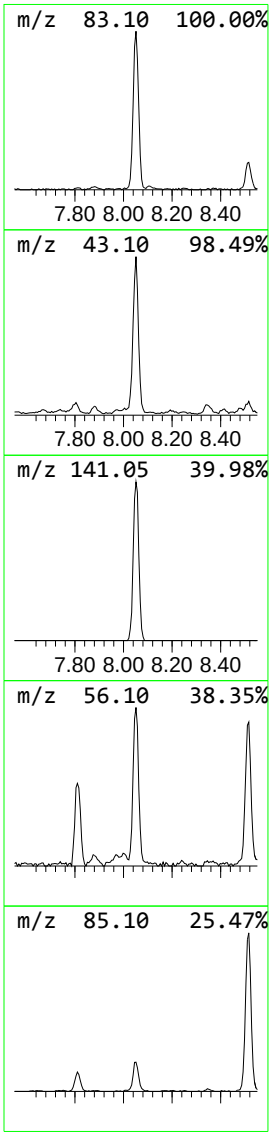
****

Peak Number 3 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	3.24 ng/ul	218497	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	43
2	1H-1,2,4-Triazole, 3-methyl-	83	C3H5N3	007170-01-6	37
3	Tetrahydropyrrolo[2,1-c][1,4]oxa...	141	C7H11NO2	101250-37-7	37
4	1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	32
5	(Trimethylsilyl)acetylene	98	C5H10Si	001066-54-2	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM093024\
Data File : BM047722.D
Acq On : 30 Sep 2024 18:34
Operator : RC/JU
Sample : P4018-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DDCE2

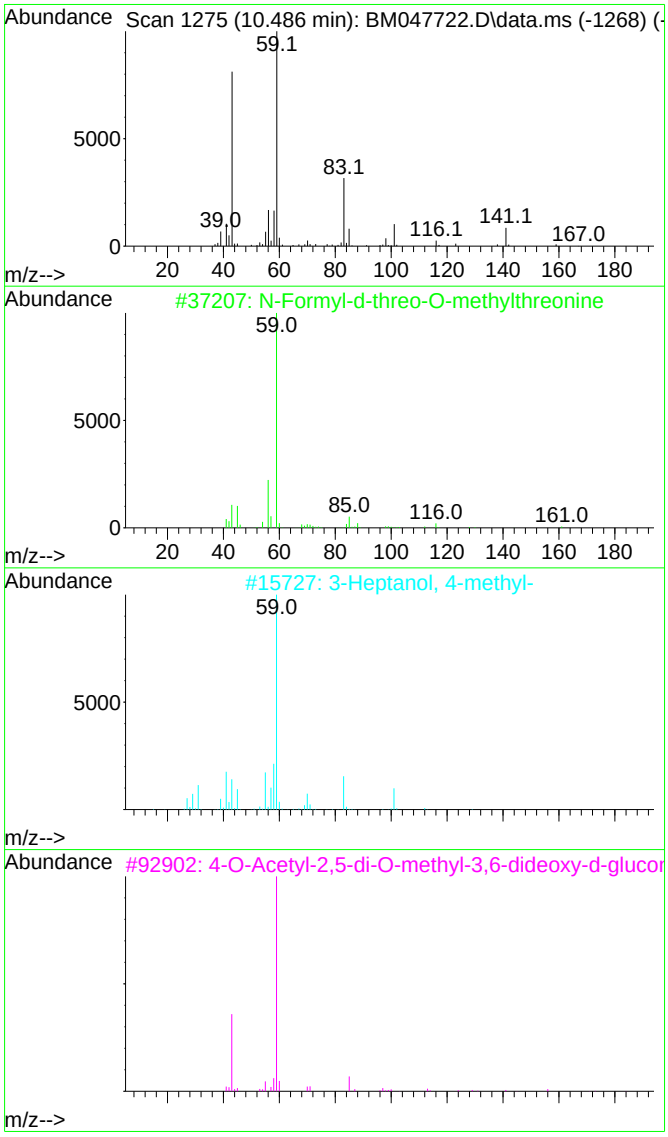
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM092724.MA.M
Quant Title : SVOA CALIBRATION

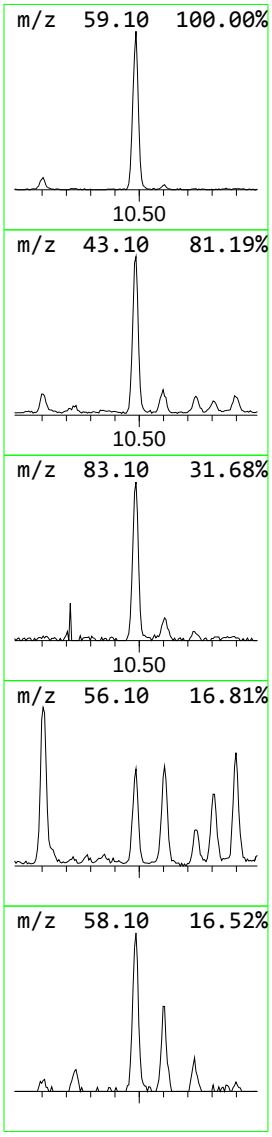
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 unknown-02 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.486	2.45 ng/ul	241328	Naphthalene-d8	10.604

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-Formyl-d-threo-O-methylthreonine	161	C6H11NO4	1000214-69-5	43
2	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	42
3	4-O-Acetyl-2,5-di-O-methyl-3,6-d...	215	C10H17NO4	1010101-80-3	40
4	Ether, hexyl t-butyl	158	C10H22O	069775-79-7	40
5	Pentane, 2-methoxy-	102	C6H14O	006795-88-6	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM093024\
Data File : BM047722.D
Acq On : 30 Sep 2024 18:34
Operator : RC/JU
Sample : P4018-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DDCE2

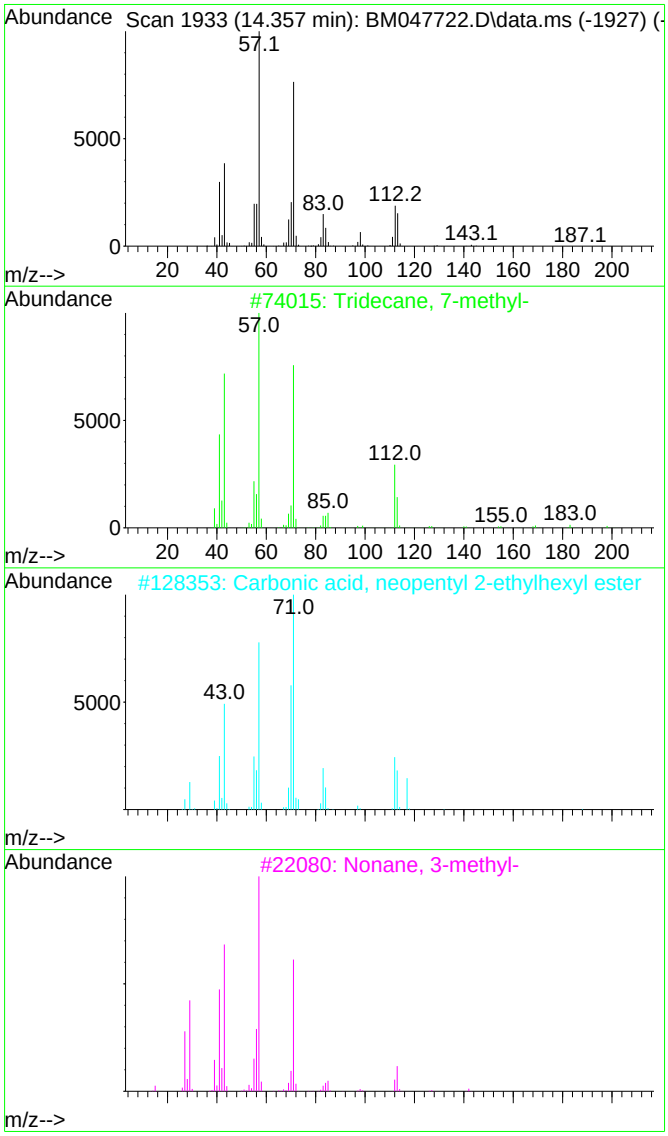
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM092724.MA.M
Quant Title : SVOA CALIBRATION

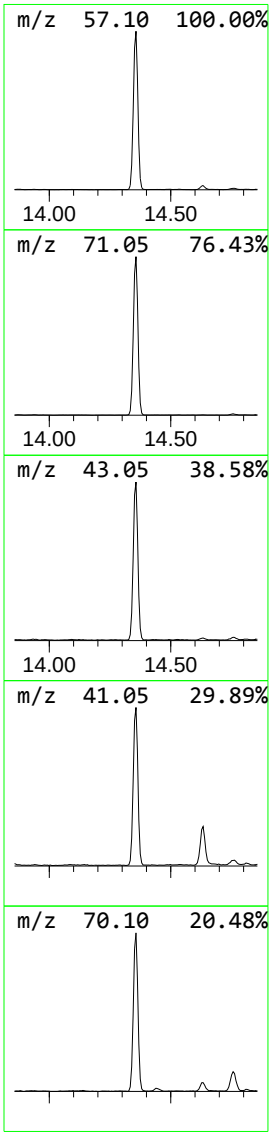
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.357	24.90 ng/ul	3104770	Acenaphthene-d10	14.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 7-methyl-	198	C14H30	026730-14-3	64
2	Carbonic acid, neopentyl 2-ethyl...	244	C14H28O3	1000357-85-7	64
3	Nonane, 3-methyl-	142	C10H22	005911-04-6	64
4	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	64
5	Octane, 2-bromo-	192	C8H17Br	000557-35-7	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM093024\
Data File : BM047722.D
Acq On : 30 Sep 2024 18:34
Operator : RC/JU
Sample : P4018-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DDCE2

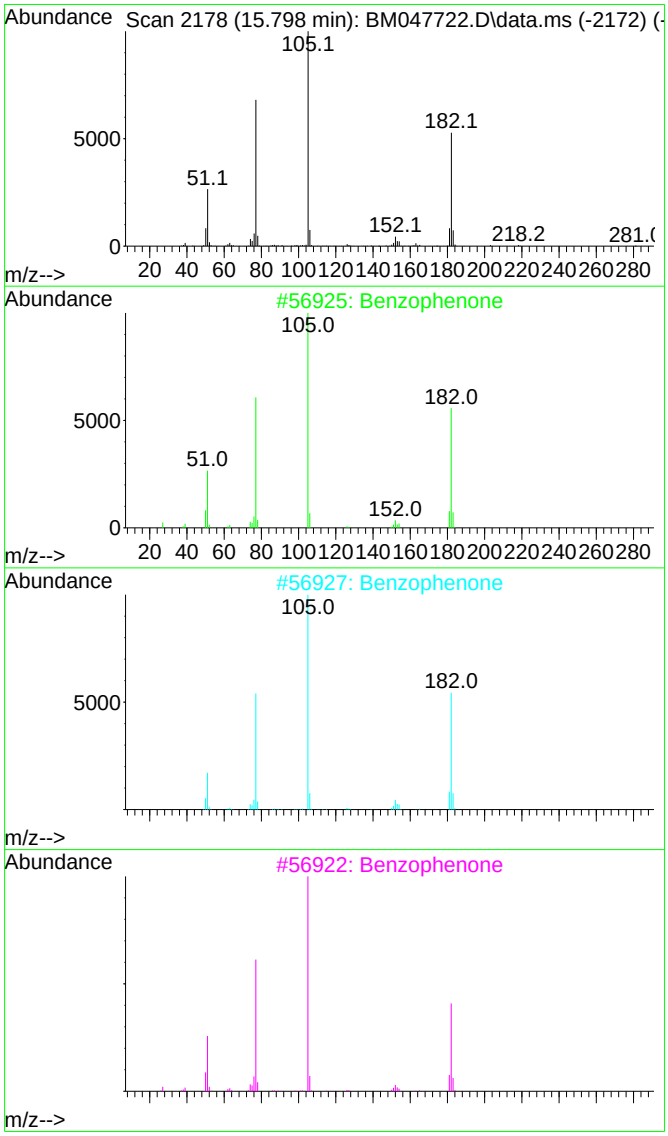
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM092724.MA.M
Quant Title : SVOA CALIBRATION

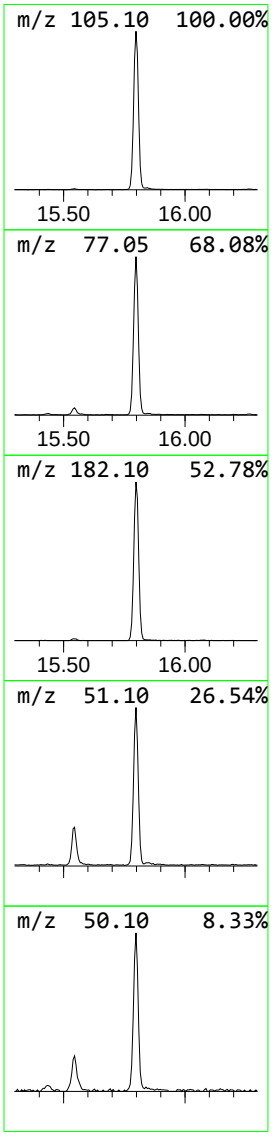
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.798	8.19 ng/ul	1021540	Acenaphthene-d10	14.445

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	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM093024\
Data File : BM047722.D
Acq On : 30 Sep 2024 18:34
Operator : RC/JU
Sample : P4018-16
Misc :
ALS Vial : 12 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

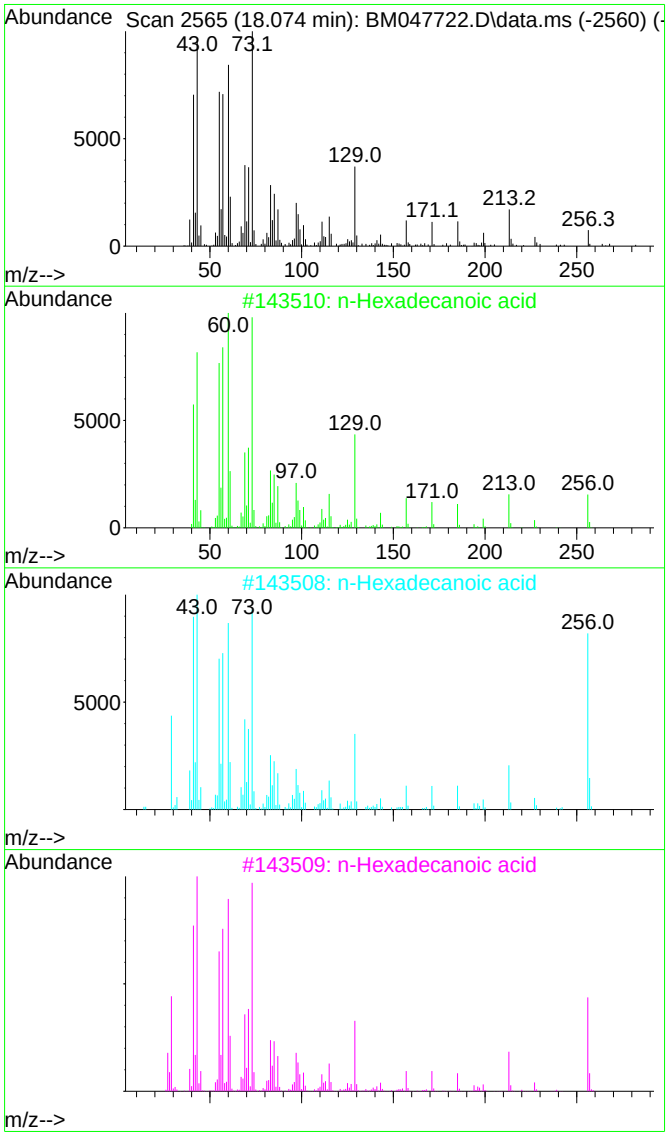
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

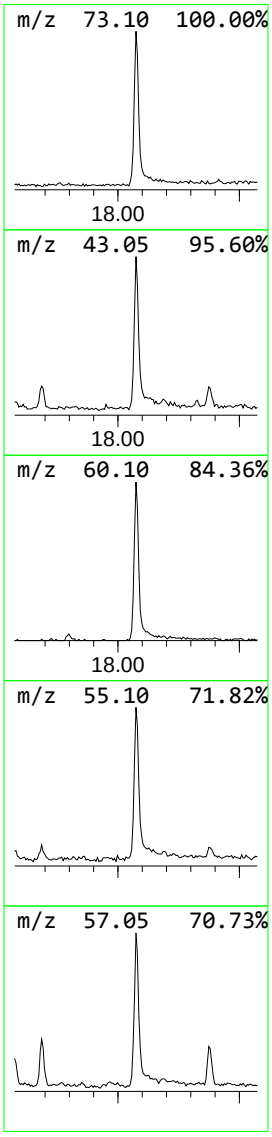
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.074	2.93 ng/ul	445411	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	99
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM093024\
Data File : BM047722.D
Acq On : 30 Sep 2024 18:34
Operator : RC/JU
Sample : P4018-16
Misc :
ALS Vial : 12 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	9.5	ng/ul	642503	1	7.810	1349900	20.0
Hexylene glycol	6.134	13.1	ng/ul	884679	1	7.810	1349900	20.0
unknown-01	8.051	3.2	ng/ul	218497	1	7.810	1349900	20.0
unknown-02	10.486	2.5	ng/ul	241328	2	10.604	1966920	20.0
(DEL) Alkane: S...	14.357	24.9	ng/ul	3104770	3	14.445	2493490	20.0
Benzophenone	15.798	8.2	ng/ul	1021540	3	14.445	2493490	20.0
n-Hexadecanoic ...	18.074	2.9	ng/ul	445411	4	17.180	3040850	20.0