LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112522\
Data File : BP012776.D
Acq On : 26 Nov 2022 19:52
Operator : CG/JU
Sample : N5602-05
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AF7

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-BP112522.M
Title : SVOA CALIBRATION

Signal : TIC: BP012776.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.399	32	36	48	rVB	139950	205930	1.18%	0.128%
2	3.669	78	82	93	rBV	790734	1077391	6.17%	0.670%
3	3.822	104	108	125	rBV	950508	1408065	8.07%	0.876%
4	4.063	144	149	162	rVB	59020	98033	0.56%	0.061%
5	4.163	162	166	171	rBV	35642	47837	0.27%	0.030%
6	5.098	317	325	333	rBV	312767	455025	2.61%	0.283%
7	7.163	668	676	686	rBV	923558	1432658	8.21%	0.891%
8	7.340	699	706	716	rBV	2130603	3358481	19.24%	2.089%
9	7.545	733	741	749	rBV	2298246	3588102	20.56%	2.231%
10	7.640	751	757	763	rVB7	14904	31820	0.18%	0.020%
11	8.016	814	821	828	rBV	1989052	3152683	18.06%	1.961%
12	8.081	828	832	837	rVB3	20228	32218	0.18%	0.020%
13	8.716	932	940	952	rBV	2427718	3905587	22.38%	2.429%
14	9.104	997	1006	1011	rBV5	15203	34558	0.20%	0.021%
15	9.186	1011	1020	1030	rVV	2416191	3961115	22.69%	2.463%
16	9.275	1032	1035	1041	rVB6	12878	22701	0.13%	0.014%
17	9.610	1085	1092	1096	rVB4	16895	30072	0.17%	0.019%
18	9.910	1135	1143	1151	rBV	1998459	3217741	18.44%	2.001%
19	10.445	1226	1234	1255	rBV	3751800	6205830	35.55%	3.859%
20	10.610	1255	1262	1266	rBV3	23190	36638	0.21%	0.023%
21	10.833	1292	1300	1309	rBV	2953429	4981151	28.54%	3.098%
22	10.969	1315	1323	1340	rBV	2465139	4399724	25.21%	2.736%
23	11.375	1386	1392	1395	rBV2	13309	24591	0.14%	0.015%
24	11.598	1424	1430	1441	rBV4	48786	155532	0.89%	0.097%
25	12.416	1562	1569	1576	rVB	68036	110996	0.64%	0.069%
26	12.639	1598	1607	1610	rBV9	8566	18990	0.11%	0.012%
27	13.263	1709	1713	1718	rVB7	11663	21568	0.12%	0.013%
28	13.545	1757	1761	1767	rVB3	28725	46832	0.27%	0.029%
29	14.057	1842	1848	1864	rBV	6797941	9807127	56.19%	6.099%
30	14.292	1885	1888	1891	rBV4	13632	21413	0.12%	0.013%
31	14.351	1891	1898	1905	rVV	8091635	12226536	70.05%	7.603%
32	14.657	1943	1950	1957	rBV	4631145	6974042	39.96%	4.337%
33	14.833	1973	1980	1986	rBV	753548	1157365	6.63%	0.720%
34	14.992	2004	2007	2009	rBV2	25407	33493	0.19%	0.021%
35	15.027	2009	2013	2016	rVV4	55092	87684	0.50%	0.055%
36	15.057	2016	2018	2022	rVB5	44384	56635	0.32%	0.035%

LSC Area Percent Report

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Acq On : 26 Nov 2022 19:52
Operator : CG/JU
Sample : N5602-05
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AF7

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-BP112522.M
Title : SVOA CALIBRATION

37	15.645	2112	2118	2127	rBV	10345246	15259687	87.43%	9.490%
38	15.757	2130	2137	2144	rBV	2748900	3842112	22.01%	2.389%
39	15.886	2156	2159	2165	rVB2	49281	71516	0.41%	0.044%
40	16.316	2229	2232	2233	rBV	80307	81755	0.47%	0.051%
41	17.410	2412	2418	2428	rBV	5817706	8097088	46.39%	5.035%
42	17.510	2429	2435	2443	rBV2	11533049	16008356	91.71%	9.955%
43	18.068	2527	2530	2537	rBV	105760	139637	0.80%	0.087%
44	18.286	2562	2567	2578	rBV	1221293	1778993	10.19%	1.106%
45	19.315	2739	2742	2748	rVB2	161858	214711	1.23%	0.134%
46	19.380	2749	2753	2766	rVV	187859	456107	2.61%	0.284%
47	19.515	2772	2776	2789	rBV	630068	904297	5.18%	0.562%
48	19.739	2808	2814	2826	rVB	12910924	17454504	100.00%	10.855%
49	21.186	3057	3060	3071	rBV	973837	1409546	8.08%	0.877%
50	21.492	3107	3112	3125	rVB	4799953	6692147	38.34%	4.162%
51	22.803	3332	3335	3342	rVB	367112	523404	3.00%	0.325%
52	23.850	3505	3513	3520	rBV2	5095983	10501474	60.16%	6.531%
53	24.009	3533	3540	3551	rVB2	2392059	4941022	28.31%	3.073%

Sum of corrected areas: 160802520

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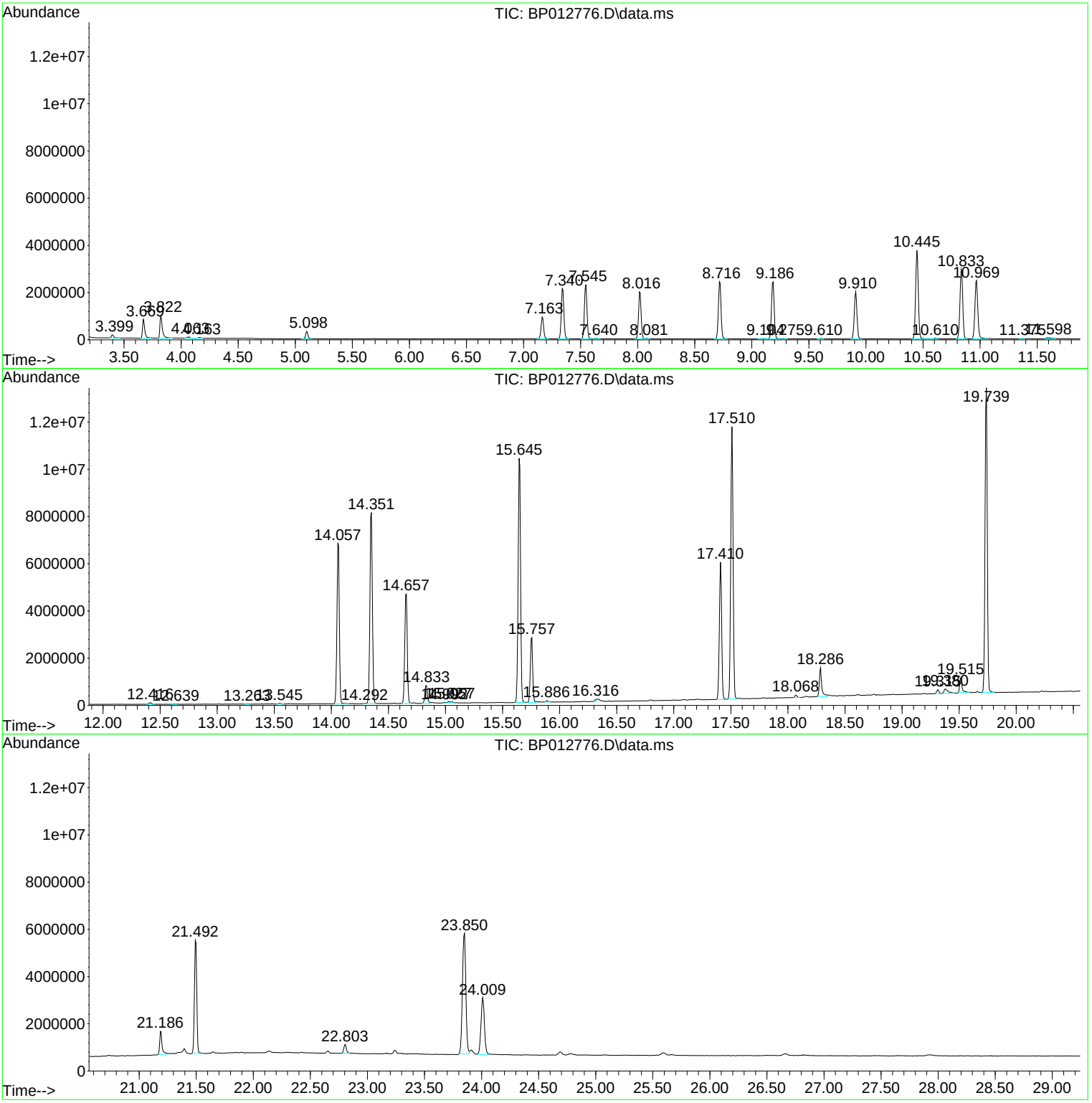
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AF7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP112522.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112522\
Data File : BP012776.D
Acq On : 26 Nov 2022 19:52
Operator : CG/JU
Sample : N5602-05
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AF7

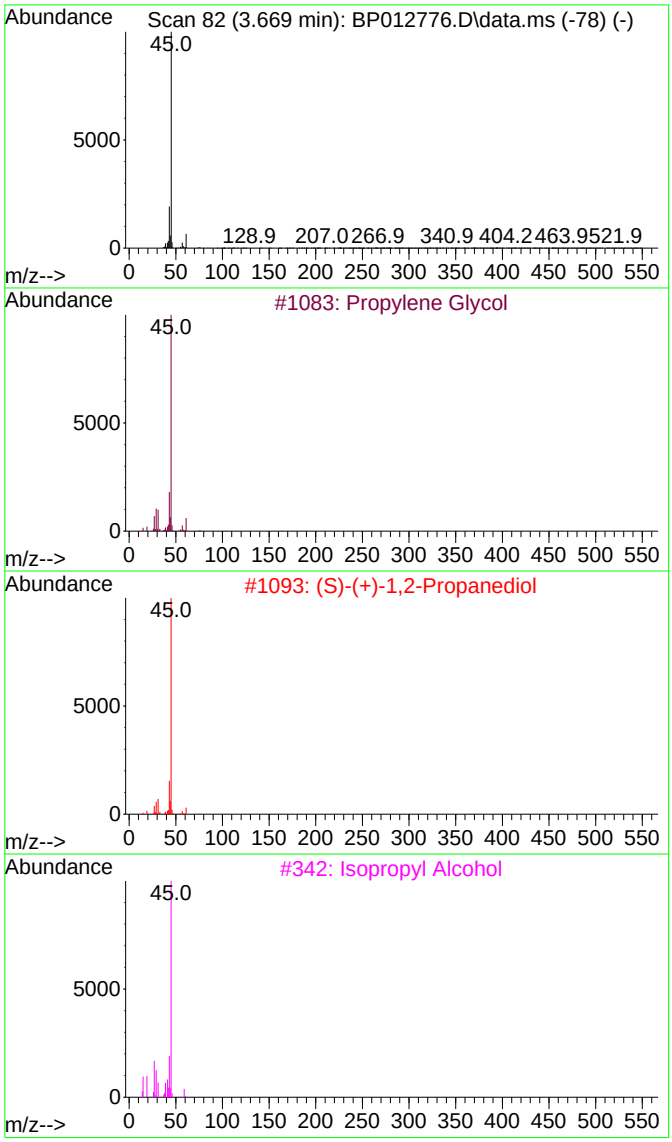
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP112522.M
Quant Title : SVOA CALIBRATION

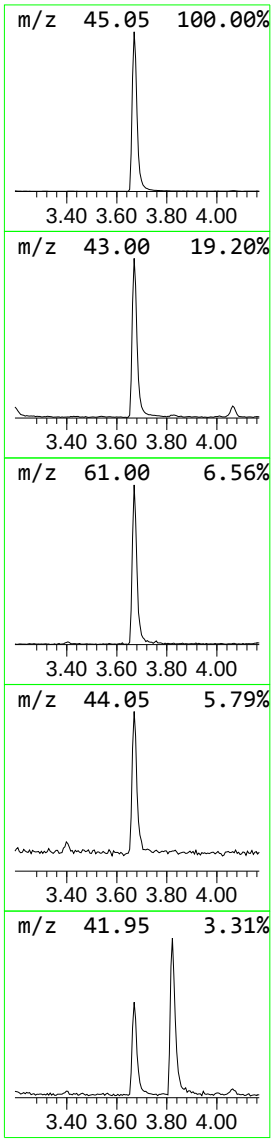
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Propylene Glycol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.669	6.83 ng/ul	1077390	1,4-Dichlorobenzene-d4	8.022

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	86
2	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5	Propylene Glycol	76	C3H8O2	000057-55-6	9





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Data File : BP012776.D
Acq On : 26 Nov 2022 19:52
Operator : CG/JU
Sample : N5602-05
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AF7

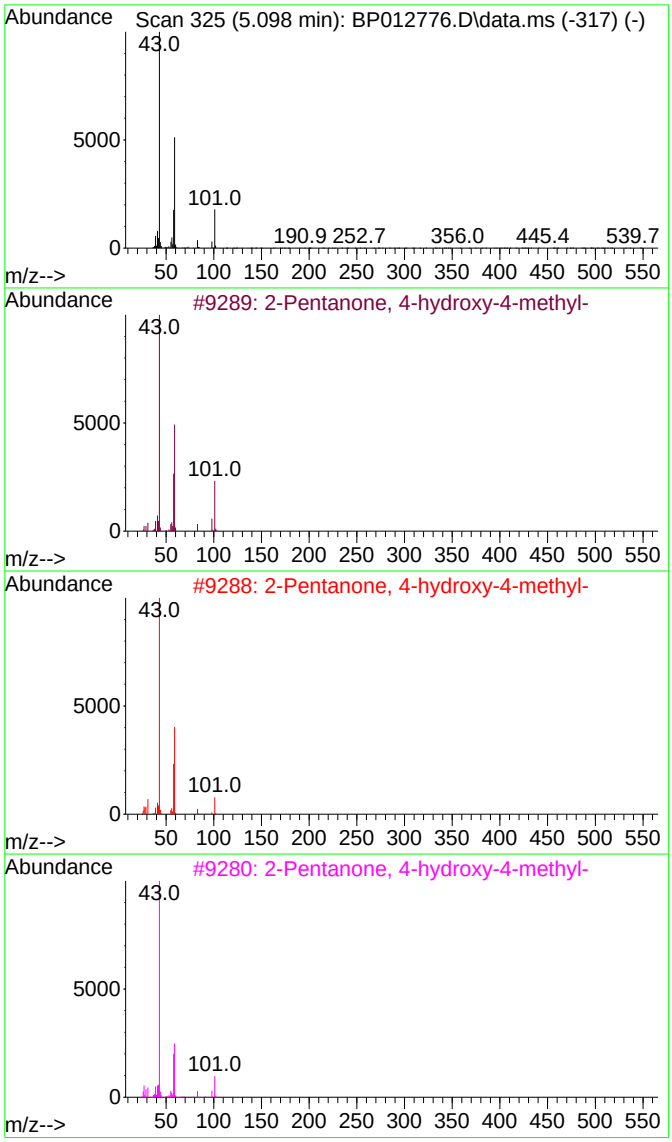
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP112522.M
Quant Title : SVOA CALIBRATION

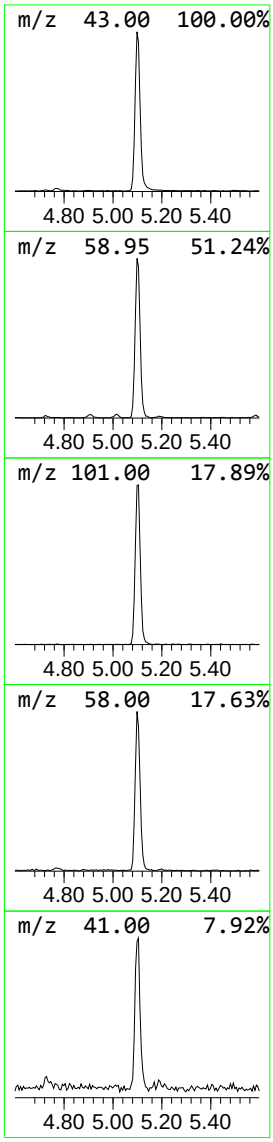
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	2.89 ng/ul	455025	1,4-Dichlorobenzene-d4	8.022

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	40
4	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112522\
Data File : BP012776.D
Acq On : 26 Nov 2022 19:52
Operator : CG/JU
Sample : N5602-05
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AF7

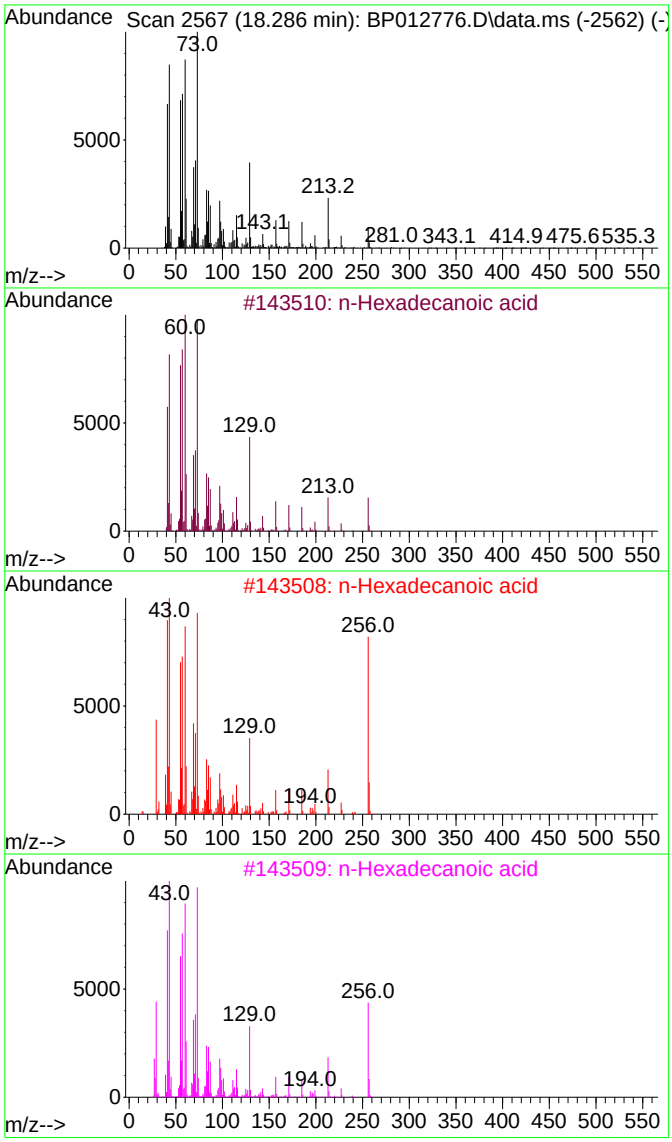
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP112522.M
Quant Title : SVOA CALIBRATION

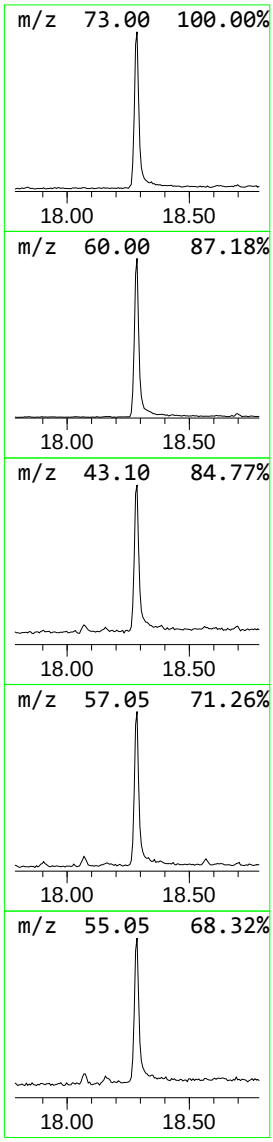
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.286	4.39 ng/ul	1778990	Phenanthrene-d10	17.410

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	98
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
5	Tridecanoic acid	214	C13H26O2	000638-53-9	95





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112522\
Data File : BP012776.D
Acq On : 26 Nov 2022 19:52
Operator : CG/JU
Sample : N5602-05
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AF7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP112522.M
Quant Title : SVOA CALIBRATION

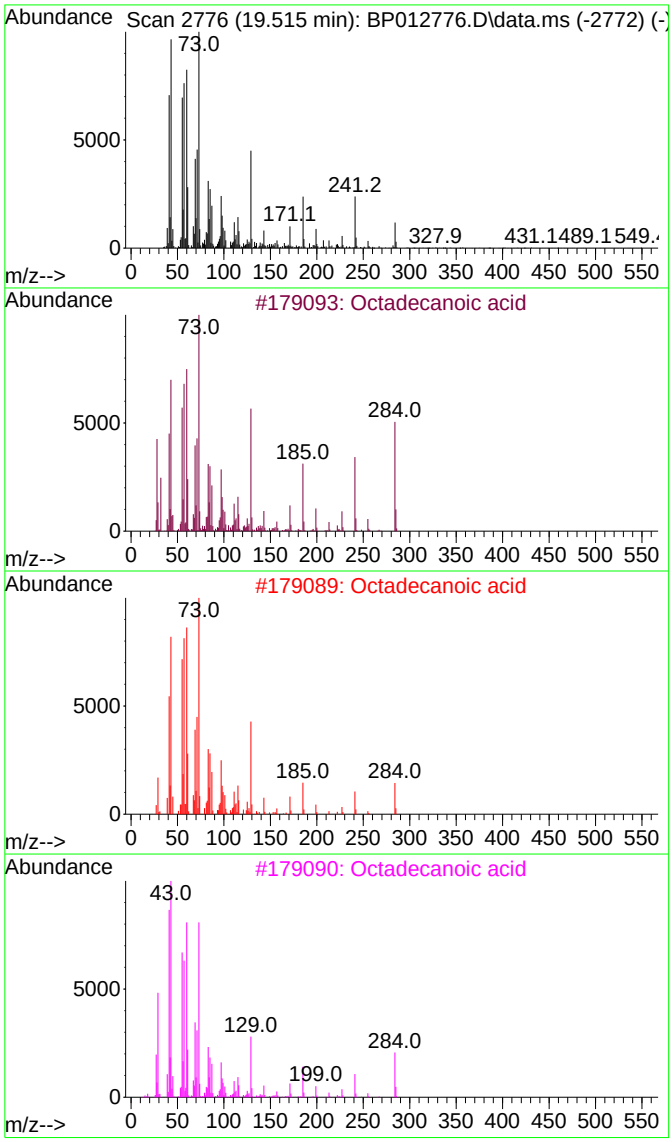
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

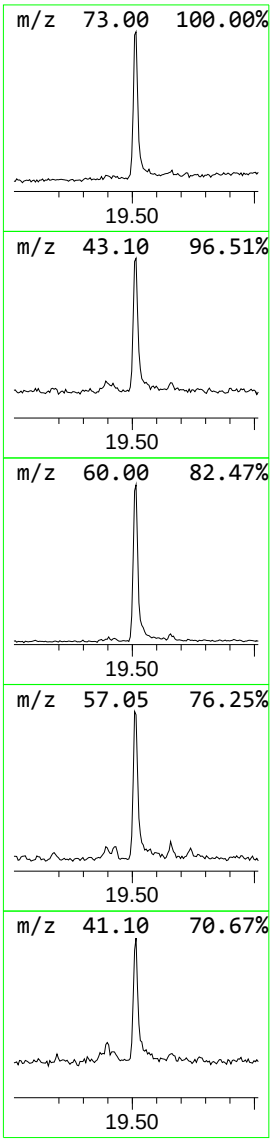
****

Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.515	2.70 ng/ul	904297	Chrysene-d12	21.492

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	99
3	Octadecanoic acid	284	C18H36O2	000057-11-4	95
4	Octadecanoic acid	284	C18H36O2	000057-11-4	94
5	Octadecanoic acid	284	C18H36O2	000057-11-4	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112522\
Data File : BP012776.D
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Sample : N5602-05
Misc :
ALS Vial : 49 Sample Multiplier: 1

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BNA_P
ClientSampleId :
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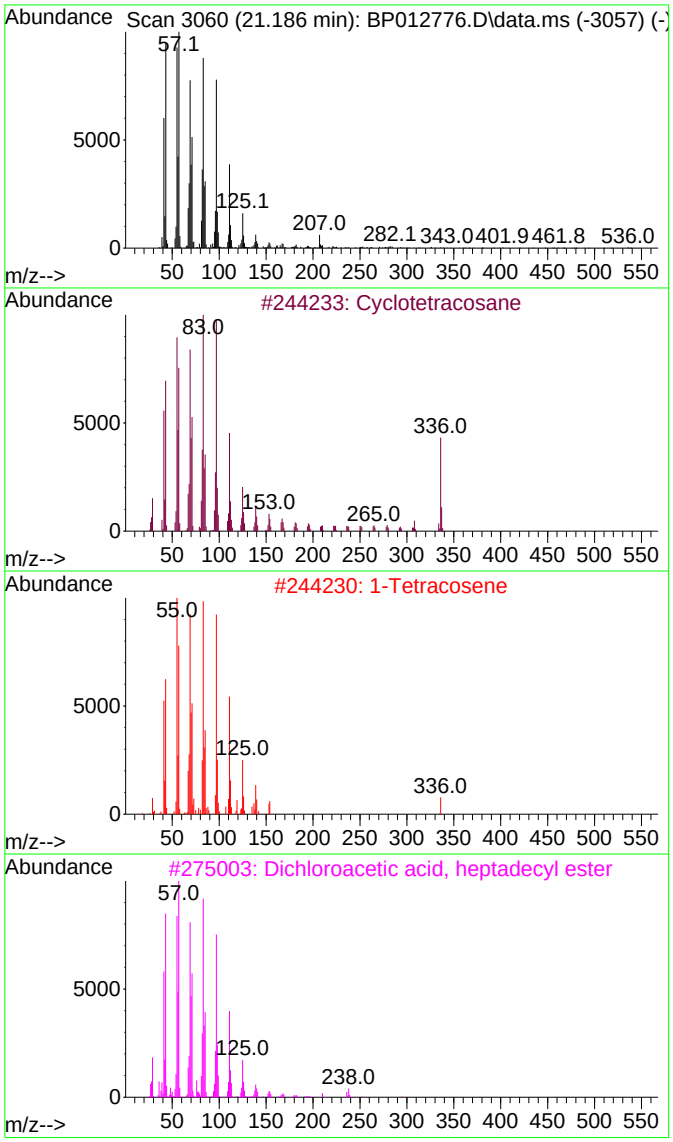
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP112522.M
Quant Title : SVOA CALIBRATION

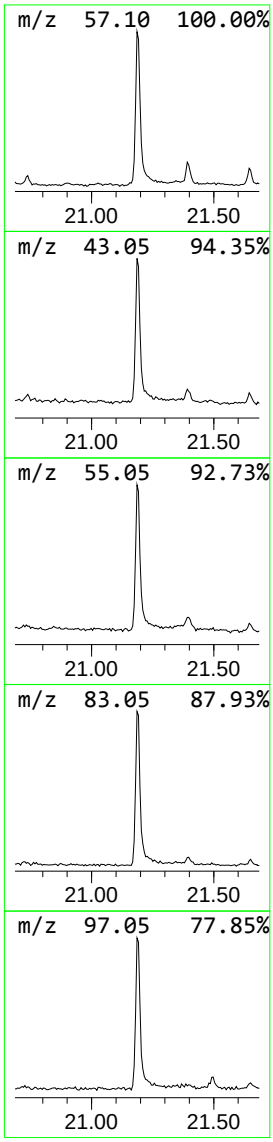
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Cyclic21.186 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.186	4.21 ng/ul	1409550	Chrysene-d12	21.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	99
2	1-Tetracosene	336	C24H48	010192-32-2	95
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	94





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BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP112522.M
Quant Title : SVOA CALIBRATION

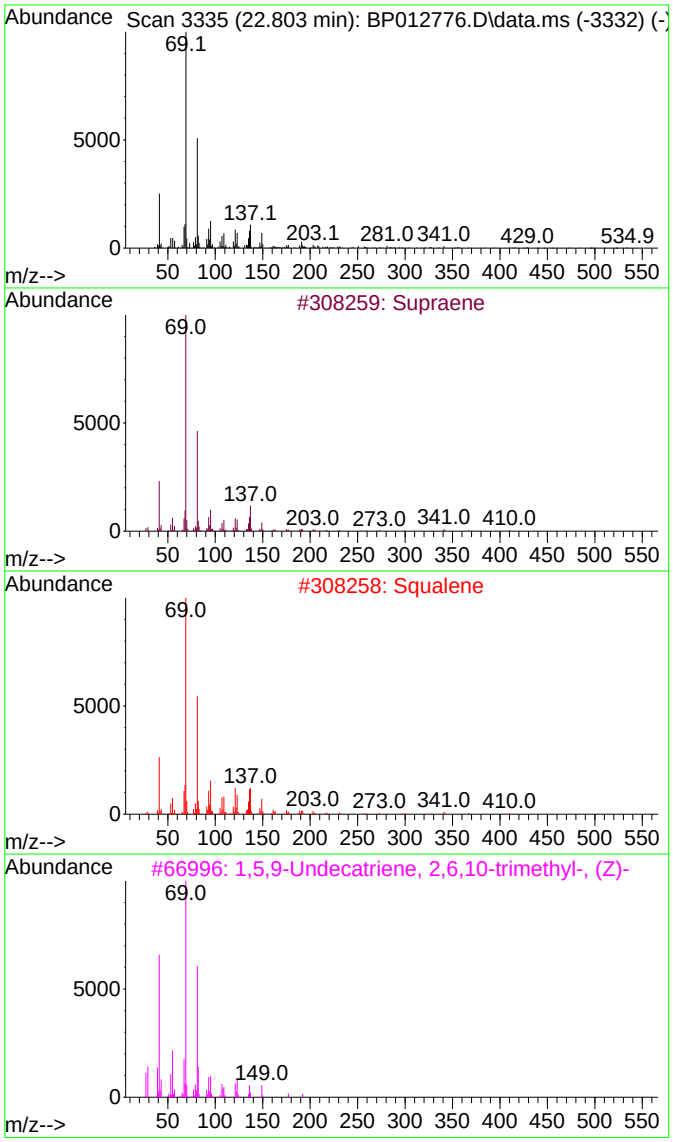
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

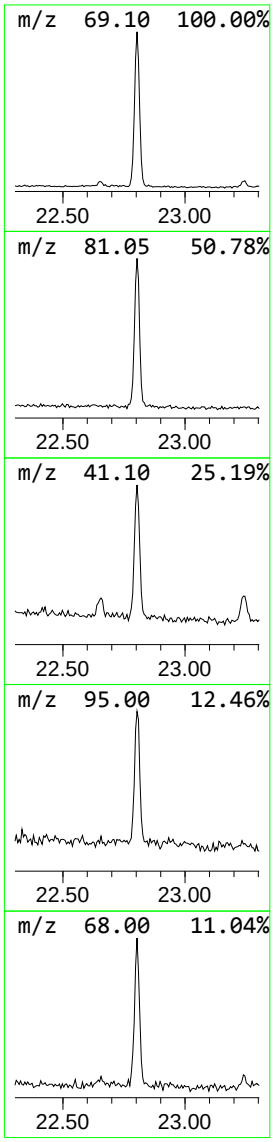
****

Peak Number 6 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.803	2.12 ng/ul	523404	Perylene-d12	24.009

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	87
2	Squalene	410	C30H50	000111-02-4	78
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	74
4	(3E,7E)-4,8,12-Trimethyltrideca-...	218	C16H26	062235-06-7	72
5	trans-Farnesol	222	C15H26O	000106-28-5	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112522\
Data File : BP012776.D
Acq On : 26 Nov 2022 19:52
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Sample : N5602-05
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP112522.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
Propylene Glycol	3.669	6.8	ng/ul	1077390	1	8.022	3152680	20.0
2-Pentanone, 4-...	5.098	2.9	ng/ul	455025	1	8.022	3152680	20.0
n-Hexadecanoic ...	18.286	4.4	ng/ul	1778990	4	17.410	8097090	20.0
Octadecanoic acid	19.515	2.7	ng/ul	904297	5	21.492	6692150	20.0
(DEL) Alkane: C...	21.186	4.2	ng/ul	1409550	5	21.492	6692150	20.0
Supraene	22.803	2.1	ng/ul	523404	6	24.009	4941020	20.0