LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062823\
Data File : BP015793.D
Acq On : 28 Jun 2023 23:28
Operator : MA/JU
Sample : 03142-21
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : DCFT8

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-BP062623.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BP015793.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.381	30	33	43	rVB	54064	75689	0.89%	0.106%
2	3.834	106	110	115	rVB3	18694	27712	0.32%	0.039%
3	3.928	123	126	135	rVB	70741	105629	1.24%	0.149%
4	4.052	142	147	150	rVB	41452	60322	0.71%	0.085%
5	4.152	159	164	174	rVB	85608	136337	1.60%	0.192%
6	4.323	191	193	198	rBV6	5785	9166	0.11%	0.013%
7	4.387	200	204	213	rVB	116348	157195	1.84%	0.221%
8	4.734	260	263	268	rVB7	9880	14002	0.16%	0.020%
9	4.817	273	277	284	rVB	45909	70305	0.82%	0.099%
10	5.122	321	329	337	rBV	286853	450219	5.28%	0.633%
11	5.222	343	346	351	rVB3	10538	15943	0.19%	0.022%
12	6.022	478	482	487	rVB8	9591	16646	0.20%	0.023%
13	6.311	527	531	535	rBV7	4428	8545	0.10%	0.012%
14	6.440	549	553	558	rBV8	4693	8624	0.10%	0.012%
15	6.911	628	633	636	rBV7	6616	11609	0.14%	0.016%
16	7.140	666	672	675	rBV8	4507	9987	0.12%	0.014%
17	7.234	681	688	707	rBV	517861	1280047	15.01%	1.800%
18	7.381	707	713	729	rVB	575395	1011888	11.87%	1.423%
19	7.587	742	748	768	rBV	718625	1338263	15.69%	1.882%
20	8.058	821	828	846	rVV	1131711	2082757	24.42%	2.929%
21	8.611	920	922	930	rVB9	5377	10894	0.13%	0.015%
22	8.793	945	953	967	rBV	513117	1192960	13.99%	1.678%
23	8.911	967	973	987	rVB	152288	327974	3.85%	0.461%
24	9.246	1022	1030	1048	rBV	621488	1279284	15.00%	1.799%
25	9.599	1086	1090	1094	rVB	11554	17906	0.21%	0.025%
26	9.975	1147	1154	1175	rBV	465646	1073331	12.59%	1.510%
27	10.258	1193	1202	1203	rBV8	11169	25262	0.30%	0.036%
28	10.358	1214	1219	1229	rVB4	13463	31641	0.37%	0.045%
29	10.540	1243	1250	1270	rBV	492622	1476306	17.31%	2.076%
30	10.887	1301	1309	1328	rVV	1563562	2991360	35.08%	4.207%
31	11.063	1332	1339	1365	rVB2	211661	709382	8.32%	0.998%
32	11.781	1459	1461	1469	rVB9	7583	13805	0.16%	0.019%
33	11.881	1472	1478	1484	rBV4	13834	27633	0.32%	0.039%
34	12.099	1508	1515	1519	rVB8	6903	14133	0.17%	0.020%
35	12.281	1542	1546	1552	rBV5	11950	21521	0.25%	0.030%
36	12.416	1562	1569	1571	rBV8	5506	10346	0.12%	0.015%

LSC Area Percent Report

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Operator : MA/JU
Sample : 03142-21
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFT8

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-BP062623.MA.M
Title : SVOA CALIBRATION

37	12.487	1577	1581	1589	rVB5	11372	22741	0.27%	0.032%
38	12.569	1589	1595	1600	rBV2	12831	27422	0.32%	0.039%
39	12.769	1625	1629	1635	rBV6	10735	20991	0.25%	0.030%
40	13.216	1700	1705	1709	rBV4	14758	24797	0.29%	0.035%
41	13.304	1716	1720	1728	rVB9	7616	13296	0.16%	0.019%
42	13.510	1749	1755	1759	rBV	28552	46338	0.54%	0.065%
43	13.581	1759	1767	1777	rVB8	18475	48875	0.57%	0.069%
44	13.687	1781	1785	1788	rVB6	7639	10314	0.12%	0.015%
45	13.881	1812	1818	1820	rBV6	10545	19629	0.23%	0.028%
46	14.028	1837	1843	1848	rBV5	25795	52289	0.61%	0.074%
47	14.116	1848	1858	1871	rBV	1411522	2373949	27.84%	3.339%
48	14.298	1887	1889	1893	rVB2	14988	17561	0.21%	0.025%
49	14.404	1900	1907	1923	rBV	1716798	2796017	32.79%	3.932%
50	14.534	1924	1929	1933	rVV4	30584	44349	0.52%	0.062%
51	14.575	1933	1936	1940	rVB2	28846	38729	0.45%	0.054%
52	14.704	1952	1958	1967	rBV	2269286	3612446	42.36%	5.081%
53	14.934	1991	1997	2001	rVB9	10483	19407	0.23%	0.027%
54	14.993	2001	2007	2016	rBV3	107287	362521	4.25%	0.510%
55	15.481	2086	2090	2094	rVV7	12372	21784	0.26%	0.031%
56	15.528	2094	2098	2105	rVB	37288	51199	0.60%	0.072%
57	15.704	2121	2128	2148	rBV	2035075	3345041	39.23%	4.705%
58	15.869	2150	2156	2180	rVV	268591	706027	8.28%	0.993%
59	16.069	2184	2190	2202	rBV	862196	1362160	15.97%	1.916%
60	16.410	2241	2248	2261	rVB3	59207	151735	1.78%	0.213%
61	16.557	2268	2273	2276	rBV6	22880	40144	0.47%	0.056%
62	16.634	2280	2286	2295	rVB	163590	264702	3.10%	0.372%
63	16.851	2319	2323	2328	rBV6	21212	29786	0.35%	0.042%
64	16.998	2345	2348	2351	rBV4	16849	21894	0.26%	0.031%
65	17.187	2377	2380	2382	rBV	42983	48584	0.57%	0.068%
66	17.339	2402	2406	2413	rVB	56385	89037	1.04%	0.125%
67	17.404	2414	2417	2422	rBV3	34376	45679	0.54%	0.064%
68	17.469	2422	2428	2433	rBV	2335871	3614104	42.38%	5.083%
69	17.510	2433	2435	2440	rVV	265186	361635	4.24%	0.509%
70	17.569	2440	2445	2457	rVB2	1706331	2843165	33.34%	3.999%
71	17.922	2503	2505	2509	rVB	36524	39625	0.46%	0.056%
72	18.134	2538	2541	2549	rVB2	128091	157444	1.85%	0.221%
73	18.263	2559	2563	2568	rBV	257329	345250	4.05%	0.486%
74	18.322	2568	2573	2581	rBV	1683286	2299463	26.96%	3.234%
75	18.592	2616	2619	2627	rBV4	72577	153024	1.79%	0.215%
76	19.198	2719	2722	2728	rBV3	97735	148034	1.74%	0.208%

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Sample : 03142-21
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFT8

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 >
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Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Title : SVOA CALIBRATION

77	19.410	2755	2758	2760	rBV	91544	106878	1.25%	0.150%
78	19.439	2760	2763	2764	rVV3	99992	125367	1.47%	0.176%
79	19.469	2764	2768	2775	rVB	679020	981766	11.51%	1.381%
80	19.545	2777	2781	2792	rBV	434345	752690	8.83%	1.059%
81	19.792	2819	2823	2836	rVB2	2225220	4194418	49.19%	5.899%
82	20.269	2902	2904	2908	rVB2	125713	138238	1.62%	0.194%
83	21.228	3062	3067	3073	rVB6	714131	1217017	14.27%	1.712%
84	21.422	3097	3100	3105	rVB	289451	293924	3.45%	0.413%
85	21.557	3117	3123	3128	rBV	1999995	3171672	37.19%	4.461%
86	22.133	3219	3221	3225	rVB	261926	273422	3.21%	0.385%
87	23.245	3405	3410	3415	rVB	1036052	1677966	19.68%	2.360%
88	23.933	3521	3527	3533	rVB2	1199723	2438478	28.60%	3.430%
89	24.098	3549	3555	3564	rBV	1425831	3261746	38.25%	4.587%
90	24.680	3649	3654	3662	rVB	1046858	2135562	25.04%	3.003%
91	28.774	4346	4350	4369	rVB3	2678559	8527590	100.00%	11.993%

Sum of corrected areas: 71102544

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Instrument :
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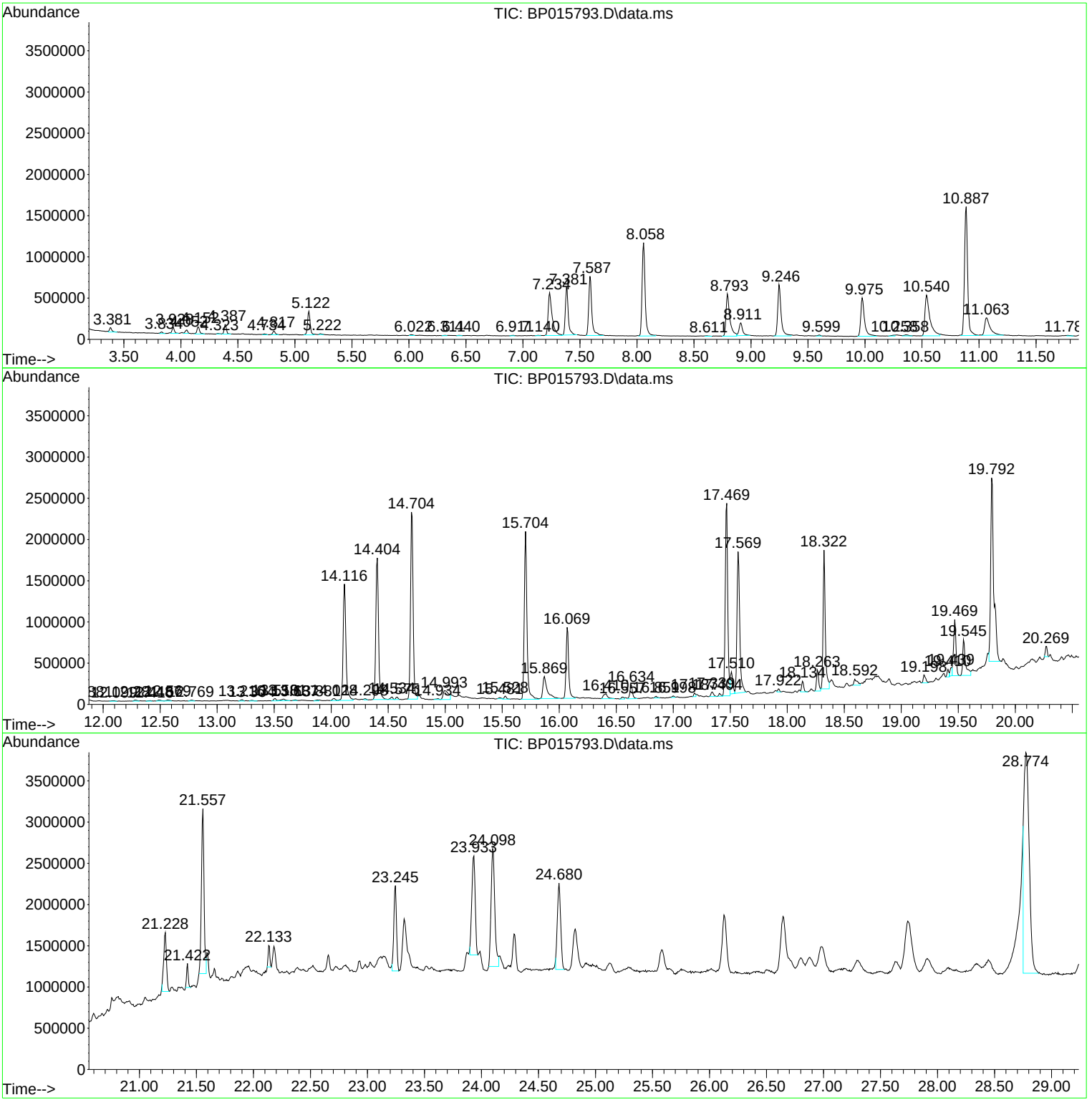
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062823\
Data File : BP015793.D
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Instrument :
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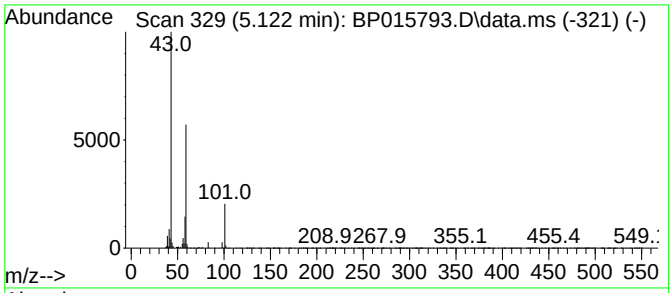
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

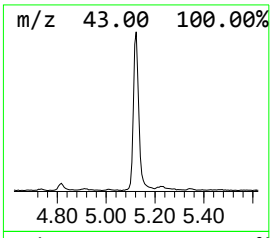
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

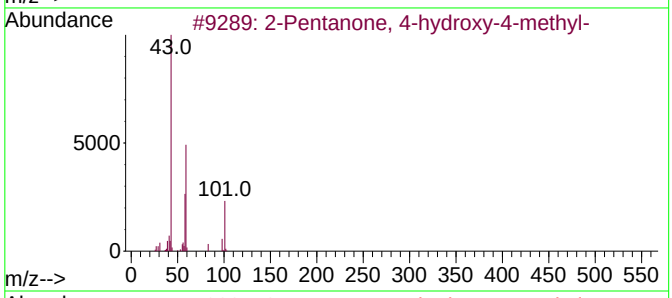
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

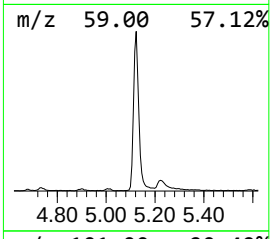
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.122	4.32 ng/ul	450219	1,4-Dichlorobenzene-d4	8.058

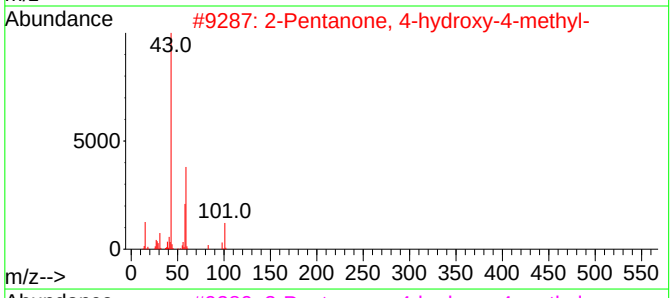
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
4	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23

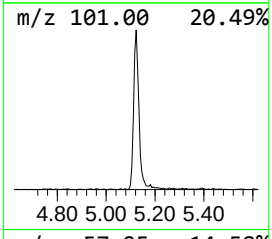


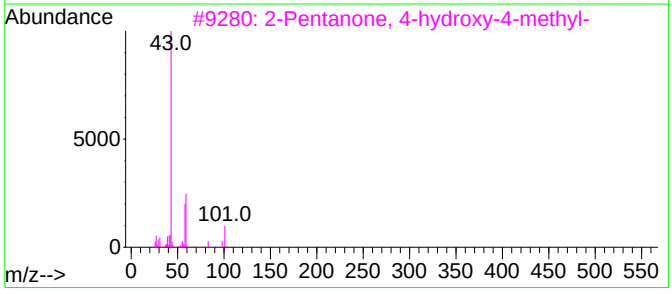


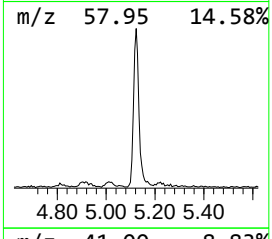


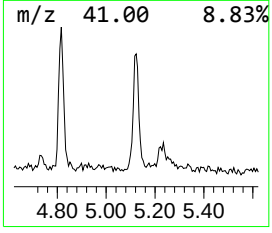












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ALS Vial : 27 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

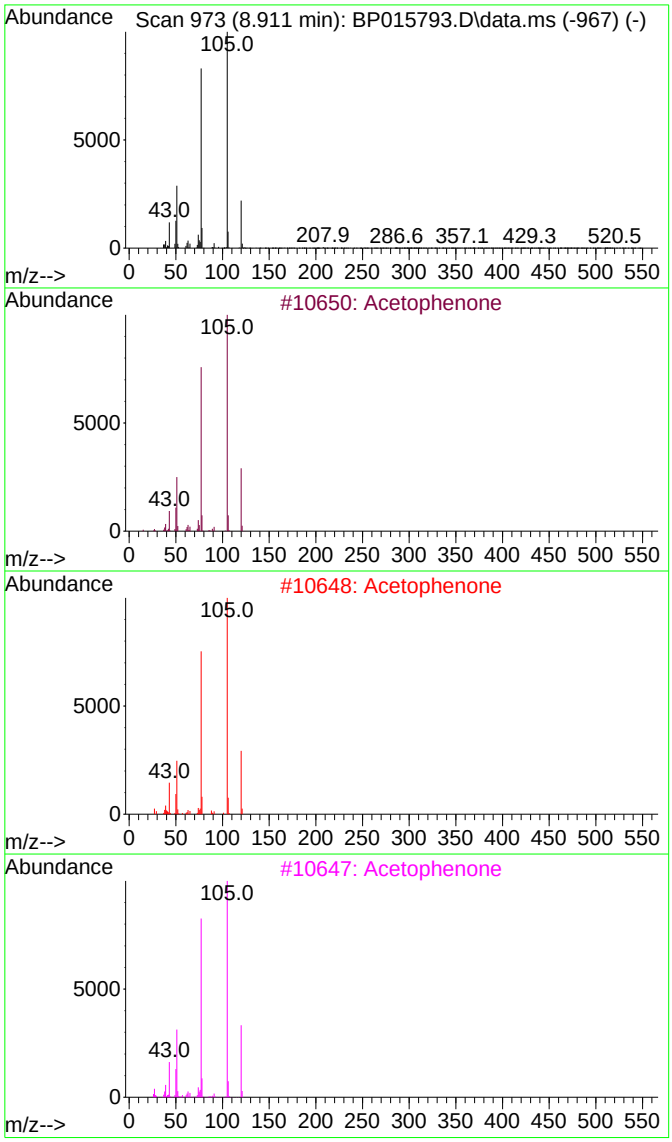
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

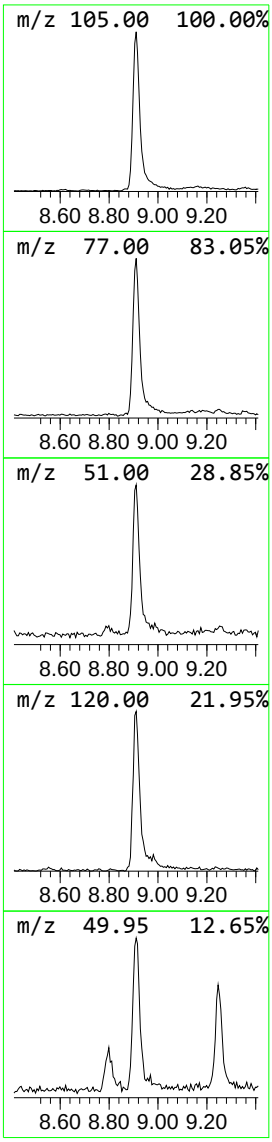
****

Peak Number 2 Aceto phenone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.911	3.15 ng/ul	327974	1,4-Dichlorobenzene-d4	8.058

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetophenone	120	C8H8O	000098-86-2	91
2	Acetophenone	120	C8H8O	000098-86-2	91
3	Acetophenone	120	C8H8O	000098-86-2	91
4	Acetophenone	120	C8H8O	000098-86-2	91
5	Acetophenone	120	C8H8O	000098-86-2	91





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

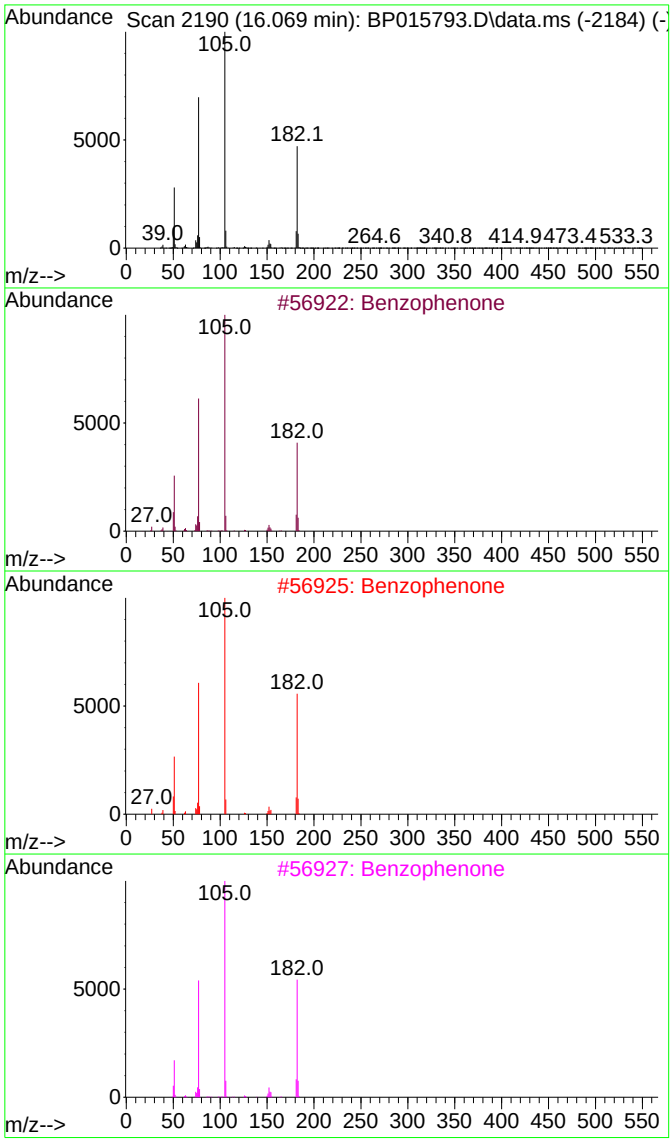
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

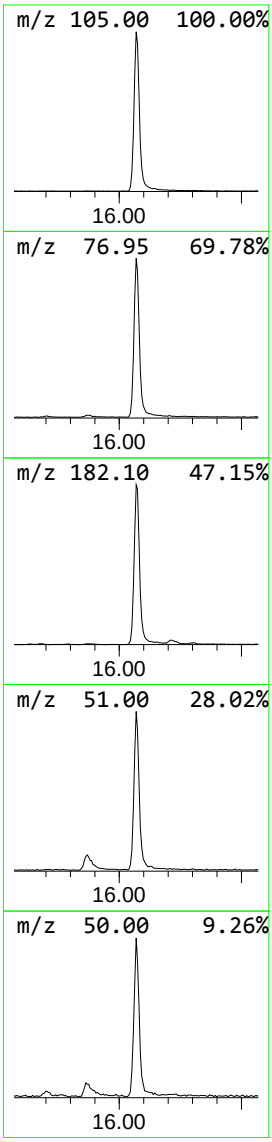
****

Peak Number 3 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.069	7.54 ng/ul	1362160	Acenaphthene-d10	14.704

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	91





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Acq On : 28 Jun 2023 23:28
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Sample : 03142-21
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFT8

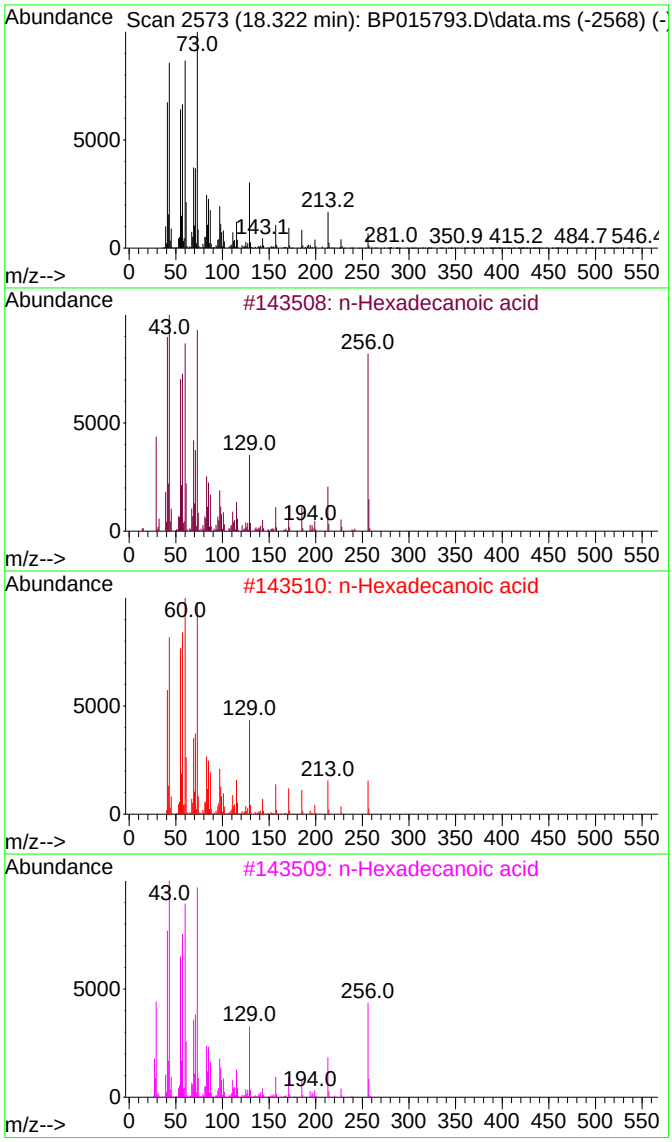
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

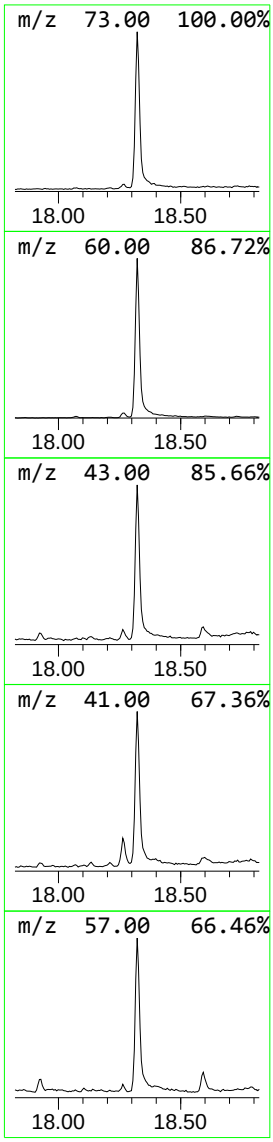
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.322	12.72 ng/ul	2299460	Phenanthrene-d10	17.469

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	96
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95





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Data File : BP015793.D
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Instrument :
BNA_P
ClientSampleId :
DCFT8

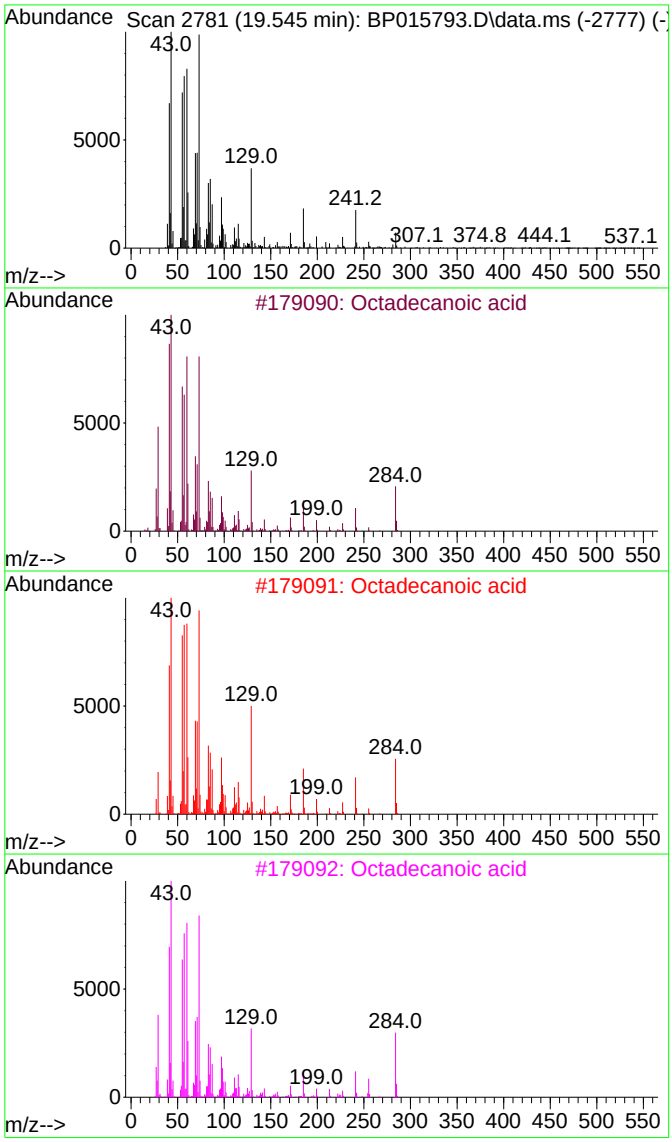
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

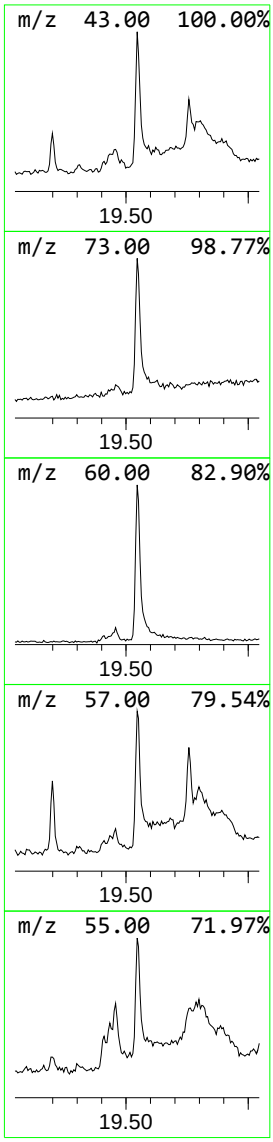
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.545	4.75 ng/ul	752690	Chrysene-d12	21.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Octadecanoic acid	284	C18H36O2	000057-11-4	98
3	Octadecanoic acid	284	C18H36O2	000057-11-4	94
4	Octadecanoic acid	284	C18H36O2	000057-11-4	94
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062823\
Data File : BP015793.D
Acq On : 28 Jun 2023 23:28
Operator : MA/JU
Sample : 03142-21
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFT8

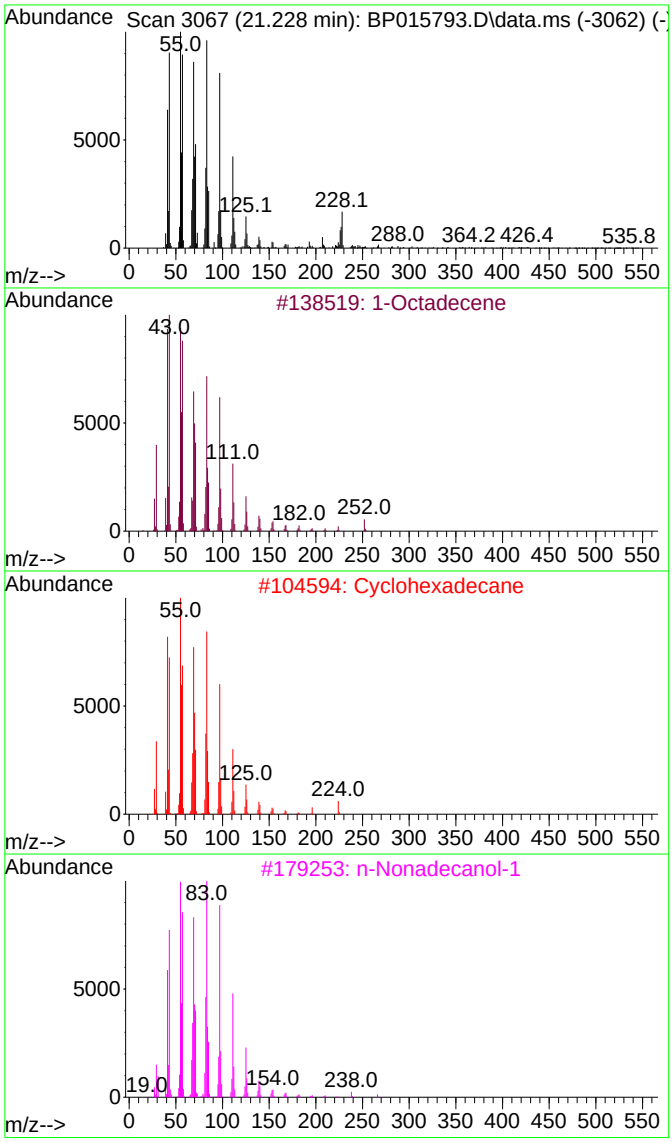
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

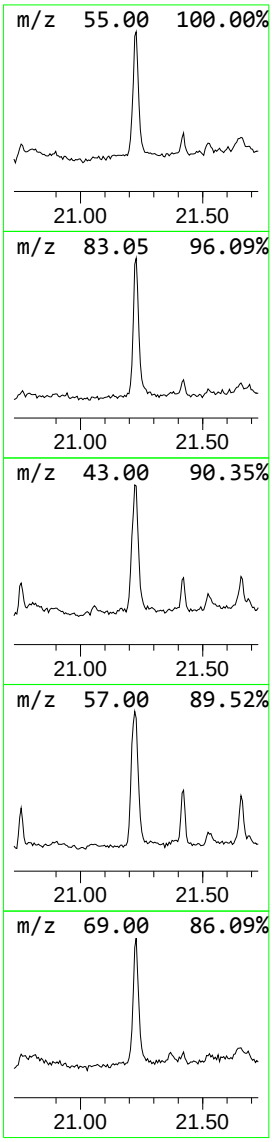
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.227	7.67 ng/ul	1217020	Chrysene-d12	21.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	96
2	Cyclohexadecane	224	C16H32	000295-65-8	94
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
4	Behenic alcohol	326	C22H46O	000661-19-8	94
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062823\
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Acq On : 28 Jun 2023 23:28
Operator : MA/JU
Sample : 03142-21
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFT8

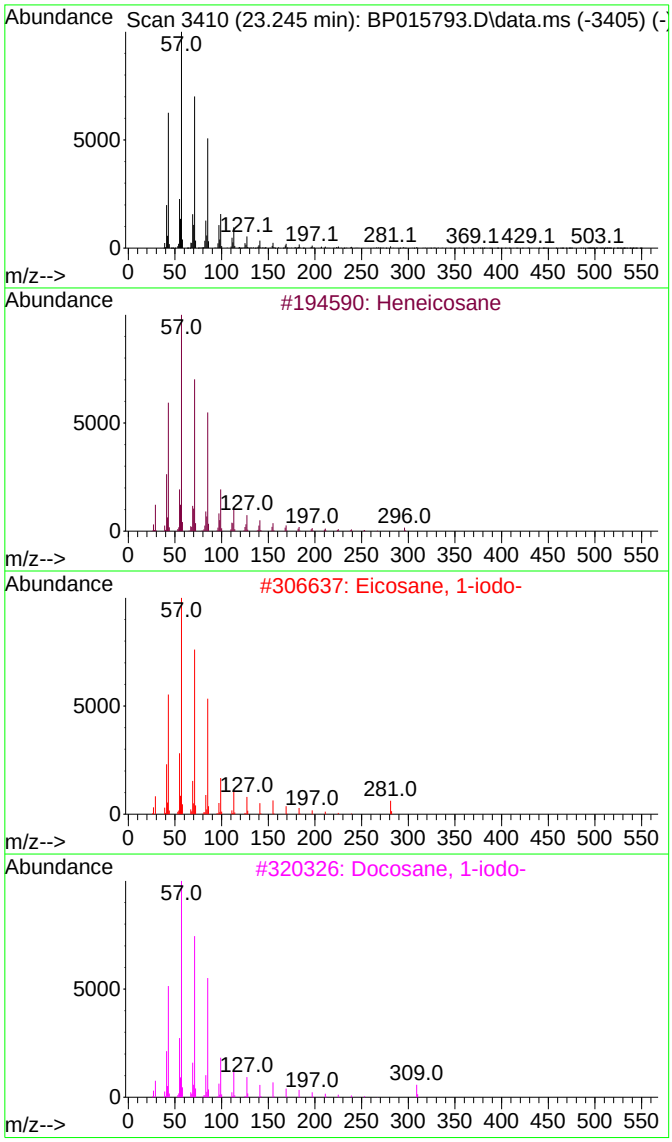
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

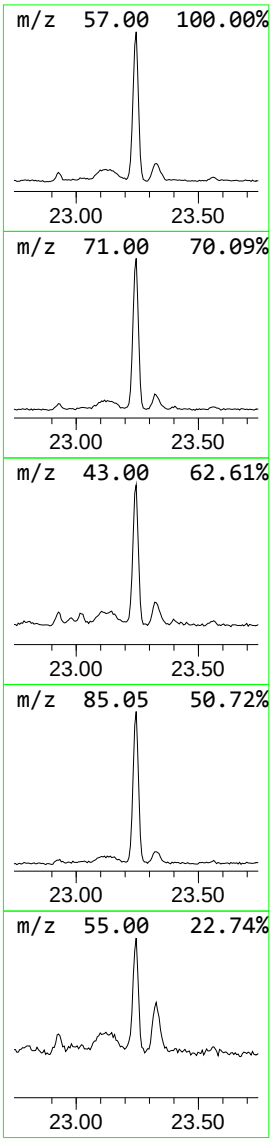
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.245	10.29 ng/ul	1677970	Perylene-d12	24.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	87
3	Docosane, 1-iodo-	436	C22H45I	1000406-31-9	87
4	Nonadecane	268	C19H40	000629-92-5	86
5	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062823\
Data File : BP015793.D
Acq On : 28 Jun 2023 23:28
Operator : MA/JU
Sample : 03142-21
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFT8

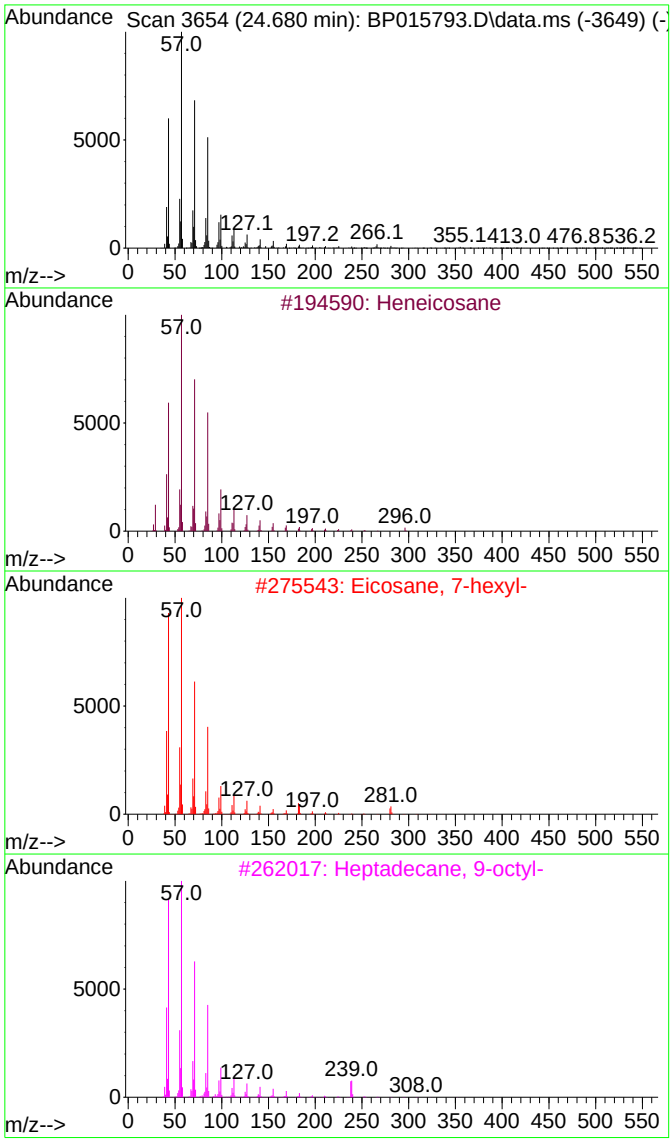
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

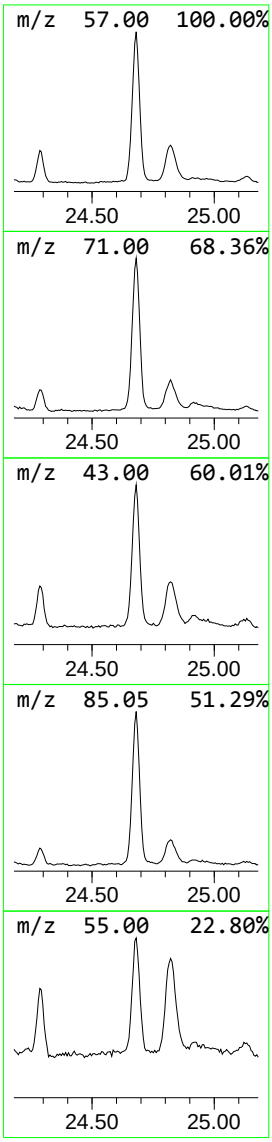
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.680	13.09 ng/ul	2135560	Perylene-d12	24.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Pentacosane	352	C25H52	000629-99-2	91
5	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062823\
Data File : BP015793.D
Acq On : 28 Jun 2023 23:28
Operator : MA/JU
Sample : 03142-21
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFT8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

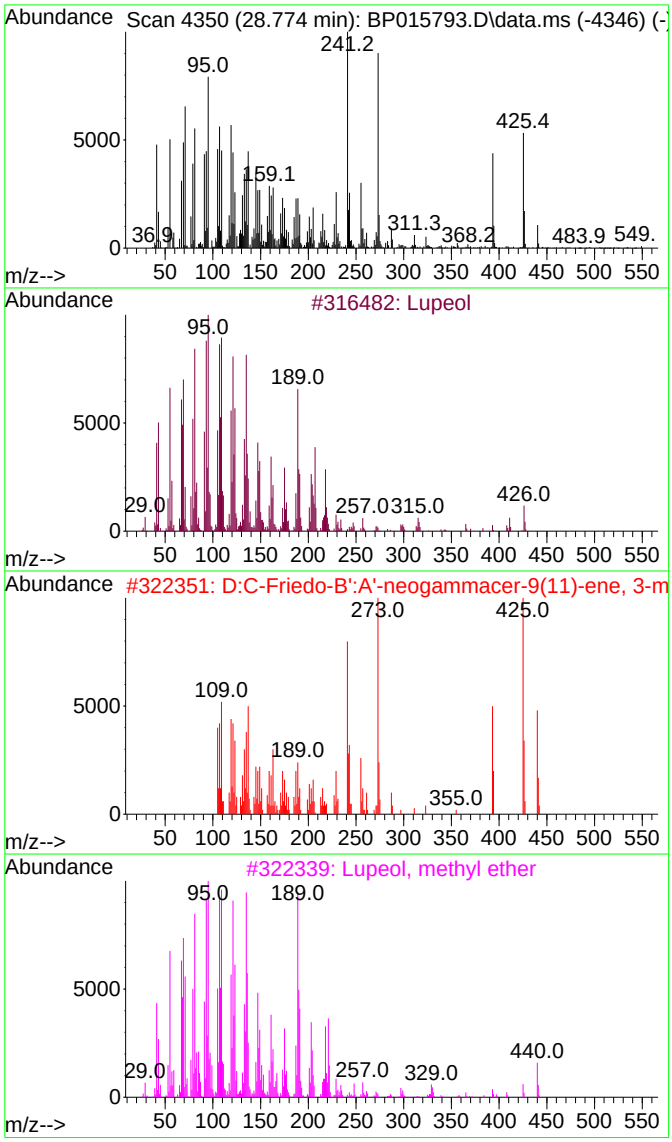
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

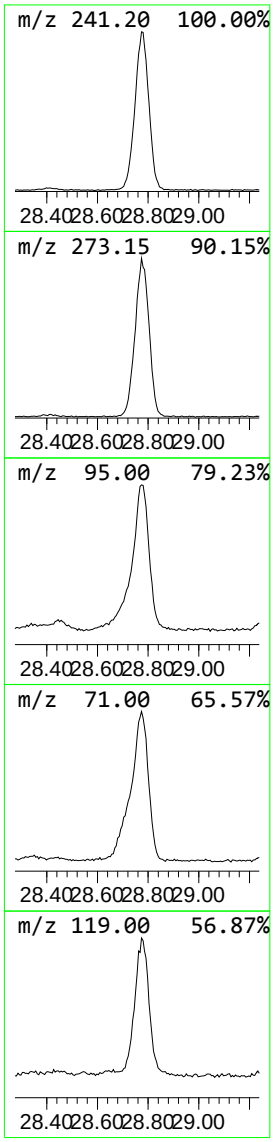
****

Peak Number 9 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.774	52.29 ng/ul	8527590	Perylene-d12	24.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lupeol	426	C30H50O	000545-47-1	44
2	D:C-Friedo-B':A'-neogammacer-9(1...	440	C31H52O	004555-56-0	35
3	Lupeol, methyl ether	440	C31H52O	025279-38-3	25
4	Pregnan-18-ol, (5.alpha.)-	304	C21H36O	056053-09-9	22
5	propanedinitrile, 2-[2-(3-methyl...	241	C11H7N5S	1000396-51-8	15





Tentatively Identified Compound (LSC) summary

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Data File : BP015793.D
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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-...	5.122	4.3	ng/ul	450219	1	8.058	2082760	20.0
Aceto phenone	8.911	3.1	ng/ul	327974	1	8.058	2082760	20.0
Benzophenone	16.069	7.5	ng/ul	1362160	3	14.704	3612450	20.0
n-Hexadecanoic ...	18.322	12.7	ng/ul	2299460	4	17.469	3614100	20.0
Octadecanoic acid	19.545	4.8	ng/ul	752690	5	21.557	3171670	20.0
(DEL) Alkane: S...	21.227	7.7	ng/ul	1217020	5	21.557	3171670	20.0
(DEL) Alkane: S...	23.245	10.3	ng/ul	1677970	6	24.098	3261750	20.0
(DEL) Alkane: S...	24.680	13.1	ng/ul	2135560	6	24.098	3261750	20.0
unknown-01	28.774	52.3	ng/ul	8527590	6	24.098	3261750	20.0