LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN061224\
Data File : BN031986.D
Acq On : 13 Jun 2024 20:53
Operator : MA/JU
Sample : P2696-13
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : A4D66

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_N\Methods\SFAM-EPA-BN052924.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BN031986.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.175	28	32	41	rVB	57749	86233	1.26%	0.112%
2	3.587	100	102	120	rBV	281529	432656	6.32%	0.564%
3	3.893	150	154	161	rVB	32262	51294	0.75%	0.067%
4	4.252	212	215	220	rVB3	23124	31588	0.46%	0.041%
5	4.722	291	295	299	rBV	7526	11405	0.17%	0.015%
6	4.793	302	307	312	rBV	21464	33348	0.49%	0.043%
7	5.181	367	373	377	rBV7	5728	10084	0.15%	0.013%
8	5.734	461	467	468	rBV	24286	34144	0.50%	0.044%
9	5.758	468	471	476	rVB	27081	44073	0.64%	0.057%
10	6.316	561	566	575	rVB2	16330	27740	0.41%	0.036%
11	6.840	646	655	664	rVB	272136	485857	7.10%	0.633%
12	6.999	675	682	697	rVB	1111131	1788483	26.13%	2.330%
13	7.193	707	715	725	rBV	1037661	1704934	24.91%	2.221%
14	7.269	726	728	736	rVV7	8084	13788	0.20%	0.018%
15	7.352	736	742	747	rVB8	5544	10071	0.15%	0.013%
16	7.657	785	794	800	rBV	1079461	1712710	25.02%	2.231%
17	7.722	800	805	817	rVB	107154	193735	2.83%	0.252%
18	7.910	832	837	841	rBV4	6930	14482	0.21%	0.019%
19	7.946	841	843	850	rVB6	6580	12148	0.18%	0.016%
20	8.157	874	879	886	rBV9	4572	10483	0.15%	0.014%
21	8.275	895	899	904	rVV6	7723	12917	0.19%	0.017%
22	8.369	908	915	922	rBV	828517	1373681	20.07%	1.789%
23	8.440	922	927	931	rVV	109060	167249	2.44%	0.218%
24	8.481	931	934	940	rVB	31069	48048	0.70%	0.063%
25	8.687	963	969	973	rBV6	6362	10508	0.15%	0.014%
26	8.752	973	980	984	rVV	59394	104953	1.53%	0.137%
27	8.816	984	991	999	rVV	1389776	2255723	32.96%	2.938%
28	8.893	999	1004	1010	rVV	72079	127731	1.87%	0.166%
29	8.975	1014	1018	1026	rVB3	22664	41224	0.60%	0.054%
30	9.151	1043	1048	1052	rBV4	10925	18323	0.27%	0.024%
31	9.204	1052	1057	1064	rVB	18950	28888	0.42%	0.038%
32	9.375	1080	1086	1092	rVB9	4926	11436	0.17%	0.015%
33	9.534	1104	1113	1118	rBV	909723	1554243	22.71%	2.025%
34	9.704	1134	1142	1149	rBV3	34993	83859	1.23%	0.109%
35	9.775	1149	1154	1158	rVB8	5673	10392	0.15%	0.014%
36	9.916	1172	1178	1188	rBV2	185622	345664	5.05%	0.450%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN061224\
Data File : BN031986.D
Acq On : 13 Jun 2024 20:53
Operator : MA/JU
Sample : P2696-13
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
A4D66

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_N\Methods\SFAM-EPA-BN052924.MA.M
Title : SVOA CALIBRATION

37	10.069	1196	1204	1217	rBV	1411383	2529311	36.96%	3.295%
38	10.228	1226	1231	1238	rVB3	34423	62287	0.91%	0.081%
39	10.298	1238	1243	1248	rVV5	18460	25964	0.38%	0.034%
40	10.351	1248	1252	1259	rVB9	14942	31643	0.46%	0.041%
41	10.440	1259	1267	1274	rBV	1496127	2577638	37.66%	3.358%
42	10.498	1274	1277	1284	rVB3	30579	47678	0.70%	0.062%
43	10.587	1284	1292	1309	rBV	1436904	2538828	37.10%	3.307%
44	10.746	1313	1319	1326	rVB10	10133	22172	0.32%	0.029%
45	10.840	1326	1335	1341	rBV8	8333	19628	0.29%	0.026%
46	10.975	1352	1358	1365	rVV2	19668	35432	0.52%	0.046%
47	11.098	1373	1379	1390	rVB	43409	92265	1.35%	0.120%
48	11.240	1397	1403	1407	rBV8	10824	21348	0.31%	0.028%
49	11.604	1461	1465	1471	rBV6	7556	15092	0.22%	0.020%
50	11.693	1475	1480	1488	rVB5	9290	14857	0.22%	0.019%
51	11.857	1504	1508	1514	rVB5	21309	36479	0.53%	0.048%
52	12.034	1528	1538	1545	rBV2	28526	58251	0.85%	0.076%
53	12.157	1554	1559	1563	rBV7	10598	20272	0.30%	0.026%
54	12.587	1626	1632	1638	rBV8	5373	12373	0.18%	0.016%
55	12.651	1638	1643	1654	rVV	38892	75836	1.11%	0.099%
56	12.904	1681	1686	1693	rBV2	58100	105167	1.54%	0.137%
57	13.145	1722	1727	1731	rBV	14103	21077	0.31%	0.027%
58	13.228	1731	1741	1755	rVB2	184253	392430	5.73%	0.511%
59	13.539	1784	1794	1797	rBV9	13642	33792	0.49%	0.044%
60	13.722	1816	1825	1838	rBV	2899080	4148544	60.62%	5.404%
61	13.834	1839	1844	1848	rVB7	14523	21690	0.32%	0.028%
62	13.998	1861	1872	1880	rBV	3332178	5073874	74.14%	6.609%
63	14.175	1897	1902	1908	rBV3	11483	21346	0.31%	0.028%
64	14.304	1916	1924	1934	rBV	2386360	3564359	52.08%	4.643%
65	14.387	1934	1938	1943	rVB2	24766	38467	0.56%	0.050%
66	14.534	1957	1963	1980	rBV	126781	273642	4.00%	0.356%
67	14.728	1990	1996	2000	rBV9	6890	14094	0.21%	0.018%
68	14.769	2000	2003	2008	rBV2	10803	16204	0.24%	0.021%
69	14.992	2035	2041	2047	rBV4	19936	36574	0.53%	0.048%
70	15.104	2056	2060	2062	rVV	13188	17992	0.26%	0.023%
71	15.134	2062	2065	2069	rVB	17029	22832	0.33%	0.030%
72	15.298	2086	2093	2105	rBV	4310438	6127535	89.53%	7.982%
73	15.434	2110	2116	2124	rVV2	276666	428407	6.26%	0.558%
74	15.539	2128	2134	2139	rVV	24992	45093	0.66%	0.059%
75	15.669	2150	2156	2162	rBV	23129	40539	0.59%	0.053%
76	16.569	2305	2309	2313	rBV3	9610	14133	0.21%	0.018%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN061224\
Data File : BN031986.D
Acq On : 13 Jun 2024 20:53
Operator : MA/JU
Sample : P2696-13
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
A4D66

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_N\Methods\SFAM-EPA-BN052924.MA.M
Title : SVOA CALIBRATION

77	16.651	2318	2323	2328	rVV4	16523	21570	0.32%	0.028%
78	16.722	2332	2335	2341	rVB7	7525	11600	0.17%	0.015%
79	16.833	2352	2354	2363	rVB4	8440	13251	0.19%	0.017%
80	17.051	2385	2391	2401	rBV	2427668	3627363	53.00%	4.725%
81	17.151	2401	2408	2417	rBV2	4683032	6844031	100.00%	8.915%
82	17.280	2427	2430	2435	rVB	20939	23973	0.35%	0.031%
83	17.339	2435	2440	2444	rBV5	17969	37634	0.55%	0.049%
84	17.439	2454	2457	2463	rBV6	7248	12415	0.18%	0.016%
85	17.727	2499	2506	2515	rBV	3292049	4461675	65.19%	5.812%
86	17.839	2522	2525	2530	rVB3	16989	23775	0.35%	0.031%
87	17.951	2540	2544	2553	rVB4	26699	41951	0.61%	0.055%
88	18.022	2553	2556	2559	rBV	14170	20453	0.30%	0.027%
89	18.163	2575	2580	2584	rBV	90775	143057	2.09%	0.186%
90	18.204	2584	2587	2592	rVB2	33683	48379	0.71%	0.063%
91	18.292	2598	2602	2605	rBV3	10497	16349	0.24%	0.021%
92	19.016	2720	2725	2732	rBV2	66294	112679	1.65%	0.147%
93	19.086	2733	2737	2741	rBV	59055	87262	1.28%	0.114%
94	19.386	2783	2788	2793	rBV2	73227	121261	1.77%	0.158%
95	19.451	2793	2799	2806	rBV2	4705353	6459187	94.38%	8.414%
96	20.392	2955	2959	2963	rBV	93523	109795	1.60%	0.143%
97	21.292	3106	3112	3118	rBV	1874389	2764921	40.40%	3.602%
98	22.645	3337	3342	3355	rVB2	570809	1104100	16.13%	1.438%
99	24.021	3568	3576	3587	rVB2	2520729	5945208	86.87%	7.745%
100	24.221	3603	3610	3622	rVB	1219022	3115505	45.52%	4.058%

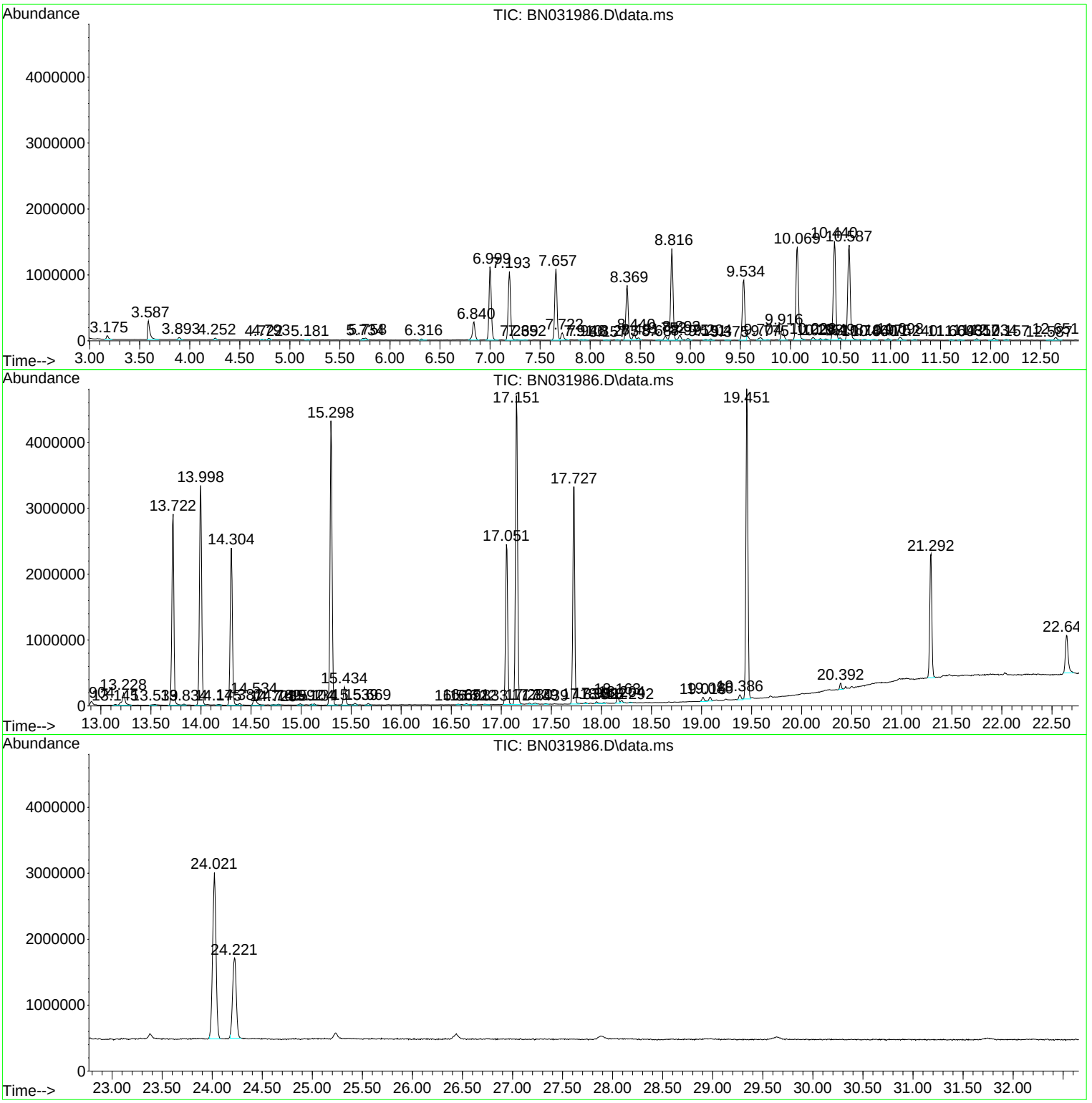
Sum of corrected areas: 76766634

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN061224\
Data File : BN031986.D
Acq On : 13 Jun 2024 20:53
Operator : MA/JU
Sample : P2696-13
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
A4D66

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN052924.MA.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN061224\
Data File : BN031986.D
Acq On : 13 Jun 2024 20:53
Operator : MA/JU
Sample : P2696-13
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
A4D66

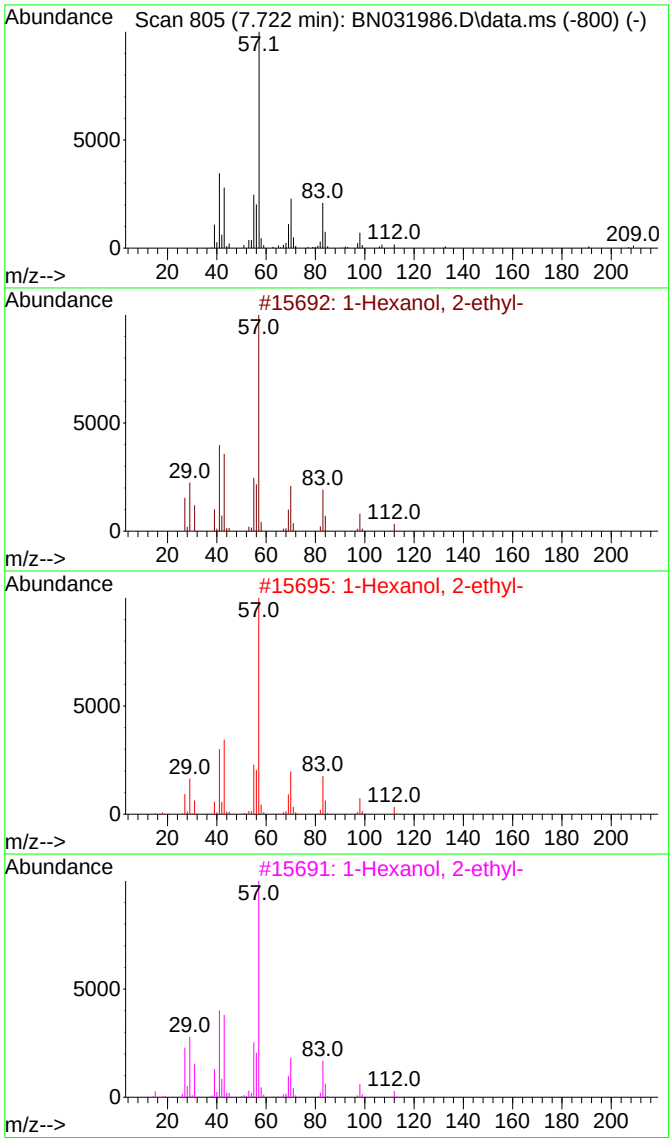
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN052924.MA.M
Quant Title : SVOA CALIBRATION

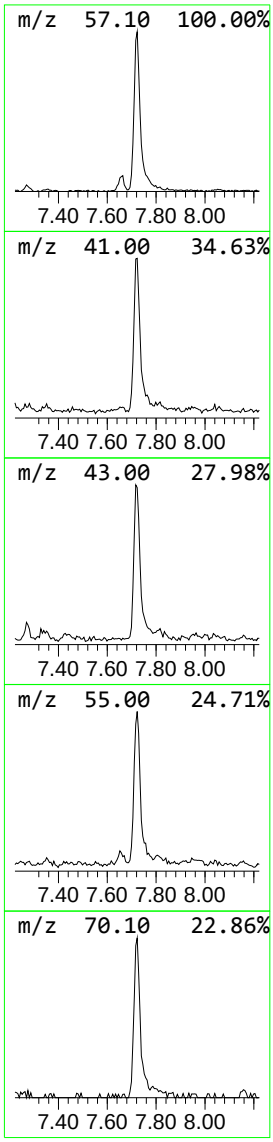
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.722	2.26 ng/ul	193735	1,4-Dichlorobenzene-d4	7.657

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN061224\
Data File : BN031986.D
Acq On : 13 Jun 2024 20:53
Operator : MA/JU
Sample : P2696-13
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
A4D66

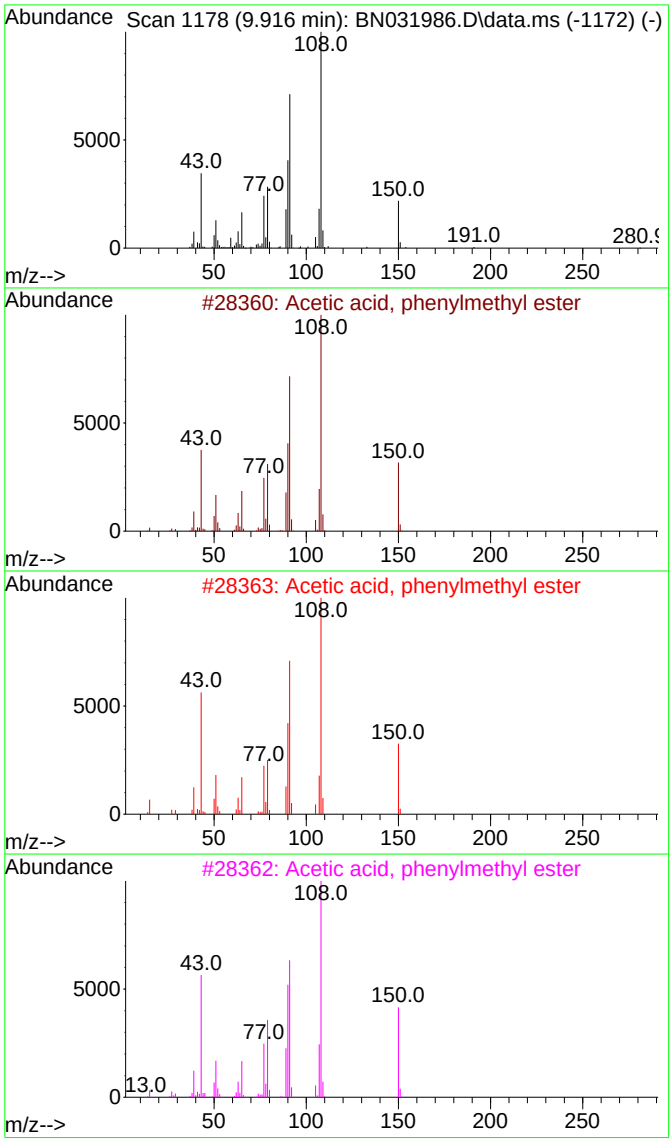
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN052924.MA.M
Quant Title : SVOA CALIBRATION

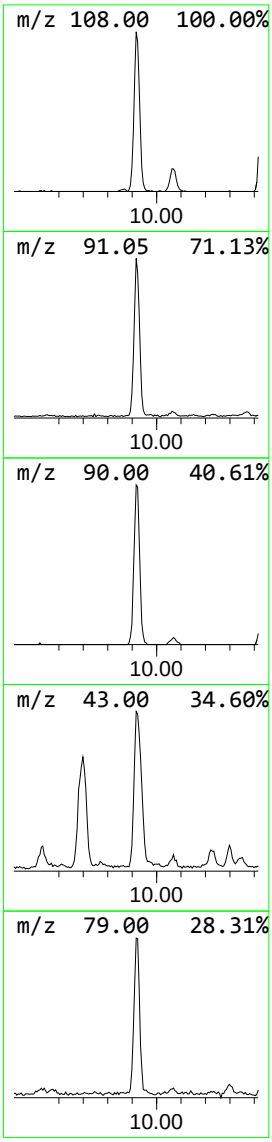
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Acetic acid, phenylmethyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.916	2.68 ng/ul	345664	Naphthalene-d8	10.440

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, phenylmethyl ester	150	C9H10O2	000140-11-4	98
2	Acetic acid, phenylmethyl ester	150	C9H10O2	000140-11-4	96
3	Acetic acid, phenylmethyl ester	150	C9H10O2	000140-11-4	96
4	Acetic acid, phenylmethyl ester	150	C9H10O2	000140-11-4	91
5	Acetic acid, phenylmethyl ester	150	C9H10O2	000140-11-4	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN061224\
Data File : BN031986.D
Acq On : 13 Jun 2024 20:53
Operator : MA/JU
Sample : P2696-13
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
A4D66

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN052924.MA.M
Quant Title : SVOA CALIBRATION

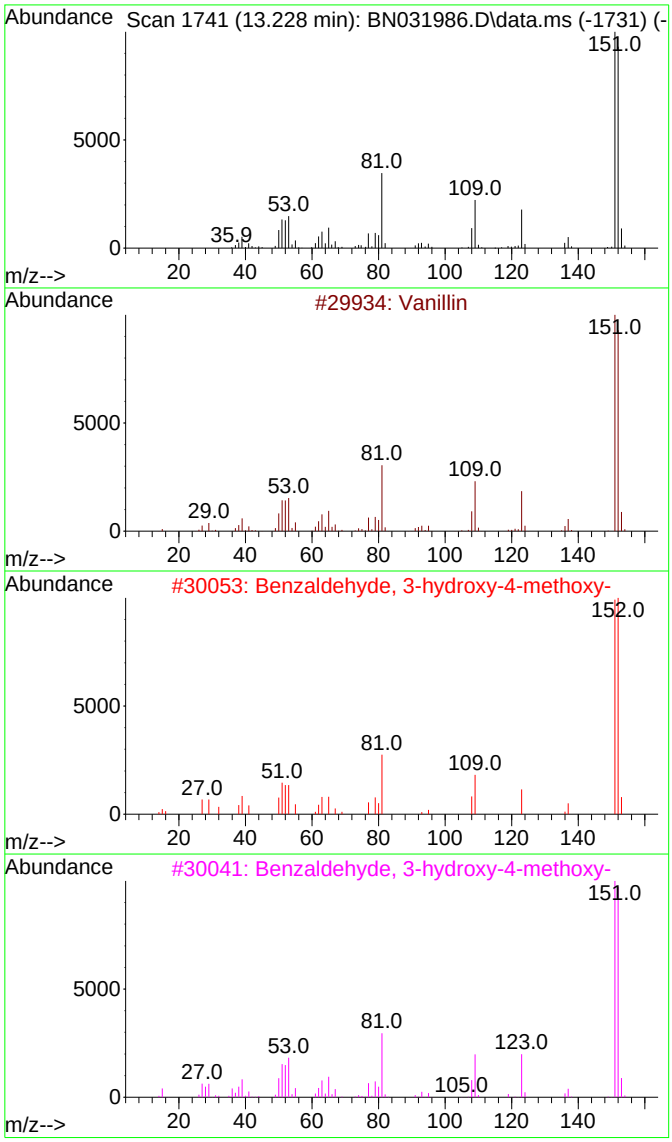
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

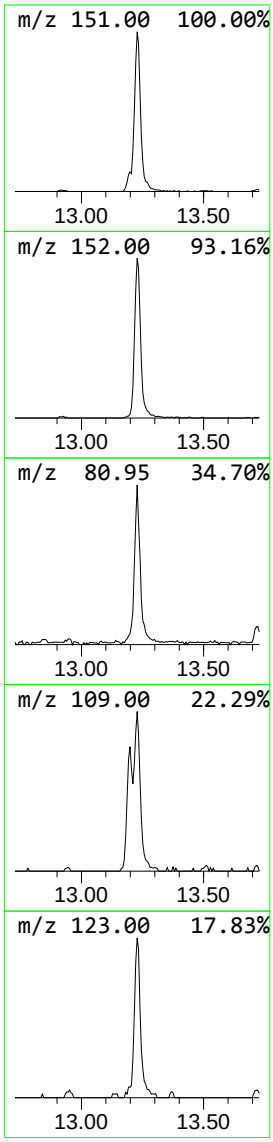
****

Peak Number 3 Vanillin Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.228	2.20 ng/ul	392430	Acenaphthene-d10	14.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Vanillin	152	C8H8O3	000121-33-5	97
2	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	97
3	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	96
4	Vanillin	152	C8H8O3	000121-33-5	96
5	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	96





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN061224\
Data File : BN031986.D
Acq On : 13 Jun 2024 20:53
Operator : MA/JU
Sample : P2696-13
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
A4D66

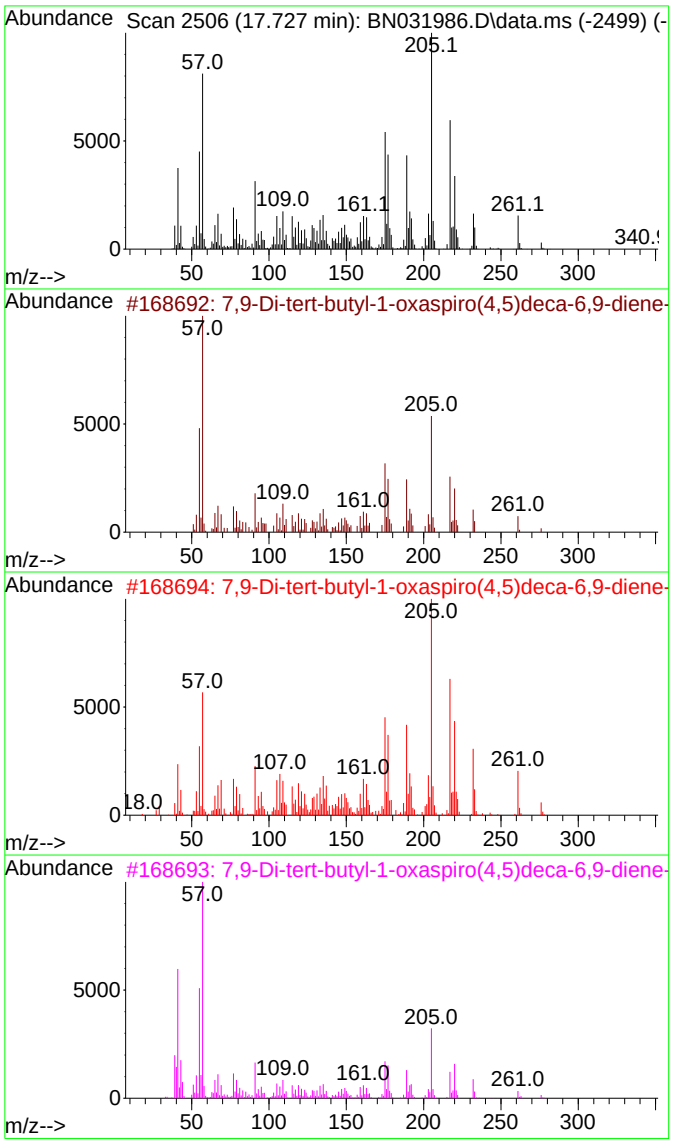
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN052924.MA.M
Quant Title : SVOA CALIBRATION

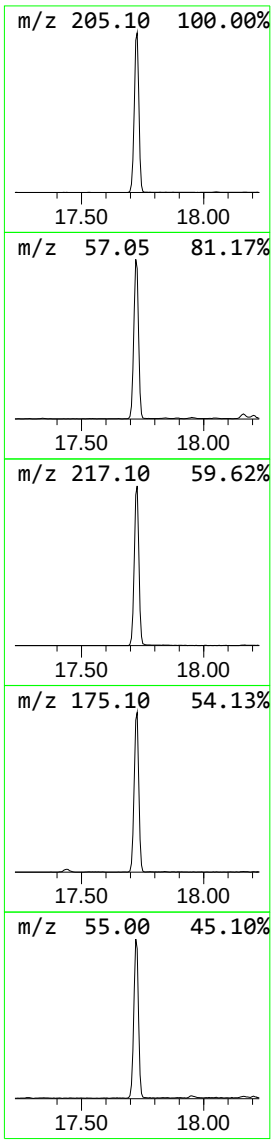
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.727	24.60 ng/ul	4461680	Phenanthrene-d10	17.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	99
2	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	95
3	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	93
4	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	50
5	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN061224\
Data File : BN031986.D
Acq On : 13 Jun 2024 20:53
Operator : MA/JU
Sample : P2696-13
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
A4D66

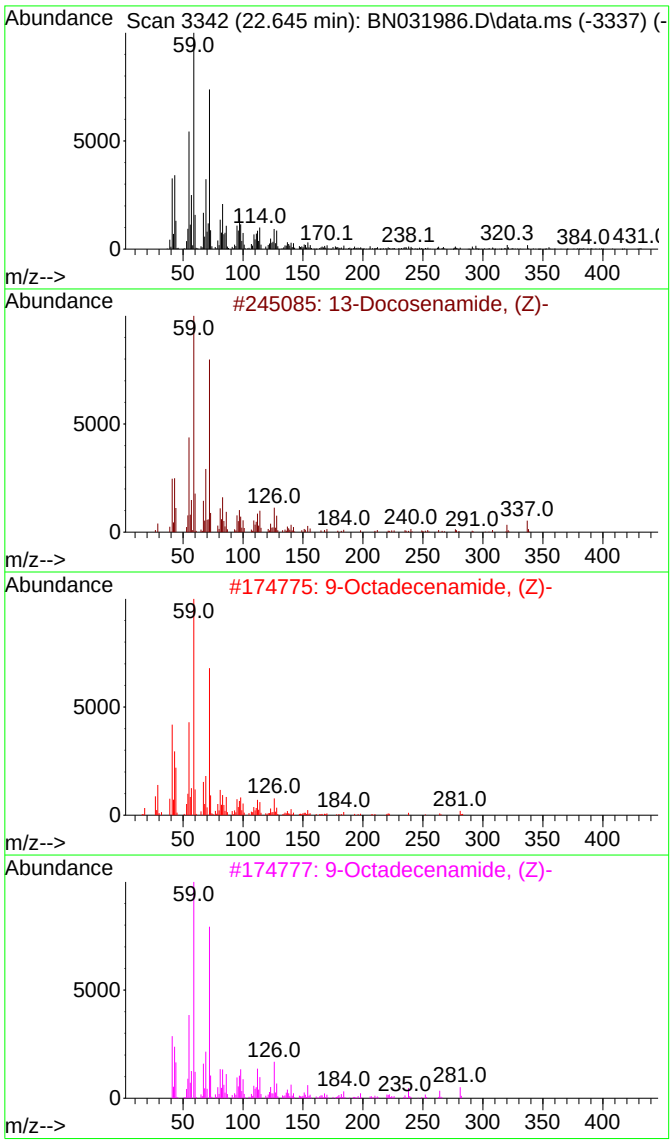
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN052924.MA.M
Quant Title : SVOA CALIBRATION

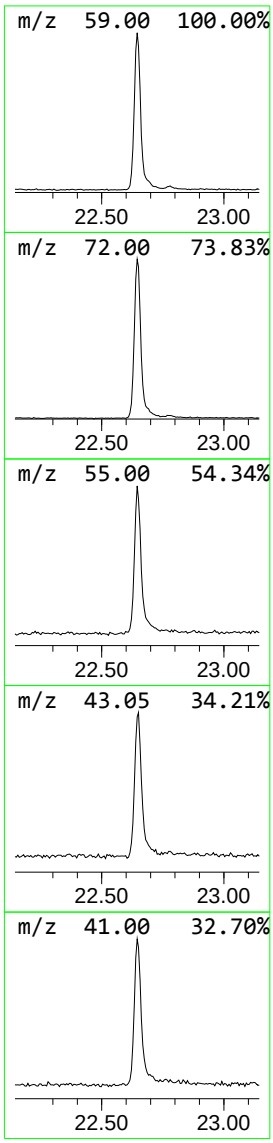
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 13-Docosenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.645	7.99 ng/ul	1104100	Chrysene-d12	21.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	98
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
3	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	95
4	9-Octadecenamide	281	C18H35NO	003322-62-1	90
5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN061224\
Data File : BN031986.D
Acq On : 13 Jun 2024 20:53
Operator : MA/JU
Sample : P2696-13
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
A4D66

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN052924.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
1-Hexanol, 2-et...	7.722	2.3	ng/ul	193735	1	7.657	1712710	20.0
Acetic acid, ph...	9.916	2.7	ng/ul	345664	2	10.440	2577640	20.0
Vanillin	13.228	2.2	ng/ul	392430	3	14.304	3564360	20.0
7,9-Di-tert-but...	17.727	24.6	ng/ul	4461680	4	17.051	3627360	20.0
13-Docosenamide...	22.645	8.0	ng/ul	1104100	5	21.292	2764920	20.0