LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102524\
Data File : BP022652.D
Acq On : 26 Oct 2024 21:24
Operator : RC/JU
Sample : P4559-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : GCNW6

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-BP100724.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BP022652.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.187	30	34	37	rBV	18569	23452	0.64%	0.088%
2	3.222	37	40	44	rVB	14337	17331	0.47%	0.065%
3	3.605	102	105	117	rBV	48185	83305	2.26%	0.312%
4	3.764	129	132	140	rVB5	5092	7558	0.21%	0.028%
5	3.911	152	157	163	rBV3	4018	8004	0.22%	0.030%
6	4.081	178	186	190	rBV10	2021	3760	0.10%	0.014%
7	4.346	226	231	236	rBV6	5287	7570	0.21%	0.028%
8	4.463	246	251	257	rBV7	3302	5422	0.15%	0.020%
9	5.022	342	346	351	rVV7	2807	5714	0.16%	0.021%
10	5.275	383	389	393	rVB9	2819	4670	0.13%	0.018%
11	5.405	404	411	416	rVB7	8271	14307	0.39%	0.054%
12	5.475	416	423	430	rBV2	23535	39469	1.07%	0.148%
13	5.634	441	450	456	rVB2	3903	10304	0.28%	0.039%
14	5.969	504	507	514	rVB9	2680	4980	0.14%	0.019%
15	6.052	514	521	525	rBV5	5241	8754	0.24%	0.033%
16	6.405	575	581	586	rBV3	2447	4205	0.11%	0.016%
17	6.793	643	647	650	rBV2	4572	6241	0.17%	0.023%
18	6.846	650	656	668	rVB	88300	147833	4.02%	0.554%
19	6.987	674	680	693	rVB	271988	405296	11.01%	1.520%
20	7.193	708	715	722	rBV	318724	497986	13.53%	1.867%
21	7.534	766	773	780	rBV	13053	21437	0.58%	0.080%
22	7.646	784	792	804	rBV	248335	413513	11.23%	1.550%
23	7.993	847	851	861	rVB5	9316	19053	0.52%	0.071%
24	8.352	905	912	924	rBV	261503	484563	13.16%	1.817%
25	8.610	946	956	966	rBV	141303	249289	6.77%	0.935%
26	8.704	966	972	979	rVB2	26852	46925	1.27%	0.176%
27	8.787	979	986	995	rBV	372264	584274	15.87%	2.191%
28	9.193	1047	1055	1064	rVB5	13790	25229	0.69%	0.095%
29	9.281	1064	1070	1077	rVB6	7795	14593	0.40%	0.055%
30	9.499	1098	1107	1119	rBV	310740	534104	14.51%	2.003%
31	9.681	1128	1138	1142	rBV8	7608	12987	0.35%	0.049%
32	9.763	1146	1152	1161	rVB8	2338	5520	0.15%	0.021%
33	9.898	1170	1175	1181	rVB7	3994	7236	0.20%	0.027%
34	10.046	1190	1200	1218	rBV	435842	840523	22.83%	3.151%
35	10.257	1232	1236	1244	rVB4	5146	10799	0.29%	0.040%
36	10.404	1250	1261	1269	rBV	359966	581090	15.78%	2.179%

LSC Area Percent Report

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Acq On : 26 Oct 2024 21:24
Operator : RC/JU
Sample : P4559-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCNW6

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-BP100724.MA.M
Title : SVOA CALIBRATION

37	10.540	1275	1284	1302	rVV	255116	491478	13.35%	1.843%
38	10.675	1302	1307	1314	rVB	3130	7877	0.21%	0.030%
39	10.810	1326	1330	1343	rVB	3535	7636	0.21%	0.029%
40	10.957	1350	1355	1360	rVB9	5475	8660	0.24%	0.032%
41	11.169	1386	1391	1393	rBV5	2867	4845	0.13%	0.018%
42	11.210	1393	1398	1404	rVV10	5484	11425	0.31%	0.043%
43	11.545	1451	1455	1460	rVB2	6606	11709	0.32%	0.044%
44	11.657	1466	1474	1480	rBV4	9462	17365	0.47%	0.065%
45	11.728	1480	1486	1487	rBV6	4253	5415	0.15%	0.020%
46	11.757	1490	1491	1496	rVV3	4302	3979	0.11%	0.015%
47	11.804	1496	1499	1506	rVB8	3665	6615	0.18%	0.025%
48	11.998	1522	1532	1535	rBV5	6610	15880	0.43%	0.060%
49	12.228	1565	1571	1574	rVV8	1818	3861	0.10%	0.014%
50	12.334	1585	1589	1593	rBV7	1990	3755	0.10%	0.014%
51	12.410	1598	1602	1608	rVB8	3642	6811	0.19%	0.026%
52	12.498	1612	1617	1621	rVB8	2955	4079	0.11%	0.015%
53	12.587	1627	1632	1643	rBV10	5265	13506	0.37%	0.051%
54	12.734	1654	1657	1661	rBV6	3044	5471	0.15%	0.021%
55	12.763	1661	1662	1672	rVB10	3802	7306	0.20%	0.027%
56	12.934	1684	1691	1696	rBV2	8484	15269	0.41%	0.057%
57	12.992	1696	1701	1707	rBV9	3274	6268	0.17%	0.024%
58	13.081	1713	1716	1722	rBV7	3025	7082	0.19%	0.027%
59	13.222	1733	1740	1747	rBV10	9580	21607	0.59%	0.081%
60	13.304	1751	1754	1761	rVV8	6086	12225	0.33%	0.046%
61	13.375	1763	1766	1771	rVB7	3222	4861	0.13%	0.018%
62	13.451	1775	1779	1784	rVB8	2372	3707	0.10%	0.014%
63	13.563	1792	1798	1803	rBV8	7459	14658	0.40%	0.055%
64	13.616	1803	1807	1808	rVV4	4527	6362	0.17%	0.024%
65	13.663	1809	1815	1836	rVB	1071226	1451235	39.42%	5.441%
66	13.875	1844	1851	1852	rBV7	2893	4496	0.12%	0.017%
67	13.951	1852	1864	1878	rVV2	963622	1463308	39.75%	5.486%
68	14.063	1878	1883	1884	rBV5	2964	3952	0.11%	0.015%
69	14.175	1898	1902	1904	rBV4	2381	3948	0.11%	0.015%
70	14.263	1910	1917	1925	rBV	557575	871264	23.67%	3.267%
71	14.439	1943	1947	1955	rVB9	6092	13290	0.36%	0.050%
72	14.522	1955	1961	1974	rBV2	58269	151445	4.11%	0.568%
73	14.734	1993	1997	2004	rVB8	8042	19193	0.52%	0.072%
74	15.057	2048	2052	2056	rBV3	10049	18497	0.50%	0.069%
75	15.098	2056	2059	2067	rVB5	9497	14738	0.40%	0.055%
76	15.269	2081	2088	2095	rBV	1345527	1960839	53.26%	7.352%

LSC Area Percent Report

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Acq On : 26 Oct 2024 21:24
Operator : RC/JU
Sample : P4559-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCNW6

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-BP100724.MA.M
Title : SVOA CALIBRATION

77	15.398	2104	2110	2122	rBV	420593	666369	18.10%	2.498%
78	15.504	2125	2128	2133	rVB6	7273	11404	0.31%	0.043%
79	15.586	2138	2142	2145	rVB5	6929	9839	0.27%	0.037%
80	15.645	2145	2152	2156	rBV	24316	36215	0.98%	0.136%
81	15.998	2209	2212	2219	rVB4	8851	15163	0.41%	0.057%
82	16.098	2227	2229	2233	rVB5	3954	4235	0.12%	0.016%
83	16.516	2297	2300	2301	rBV3	4700	4416	0.12%	0.017%
84	16.651	2318	2323	2333	rVB2	28429	45775	1.24%	0.172%
85	17.051	2385	2391	2398	rBV	864261	1200524	32.61%	4.501%
86	17.163	2402	2410	2423	rVB	1505953	2350224	63.84%	8.812%
87	17.992	2547	2551	2557	rBV	62269	82737	2.25%	0.310%
88	18.263	2595	2597	2600	rBV4	5946	7953	0.22%	0.030%
89	19.086	2734	2737	2741	rBV2	25251	31784	0.86%	0.119%
90	19.163	2746	2750	2753	rBV	27379	40934	1.11%	0.153%
91	19.204	2753	2757	2768	rVB3	67492	132180	3.59%	0.496%
92	19.327	2774	2778	2782	rBV2	50591	66865	1.82%	0.251%
93	19.539	2809	2814	2822	rBV	2526498	3086512	83.84%	11.572%
94	21.486	3139	3145	3153	rBV	989123	1600734	43.48%	6.002%
95	24.521	3651	3661	3673	rVB	1336889	3681594	100.00%	13.803%
96	24.745	3689	3699	3709	rVB2	589169	1732894	47.07%	6.497%

Sum of corrected areas: 26671564

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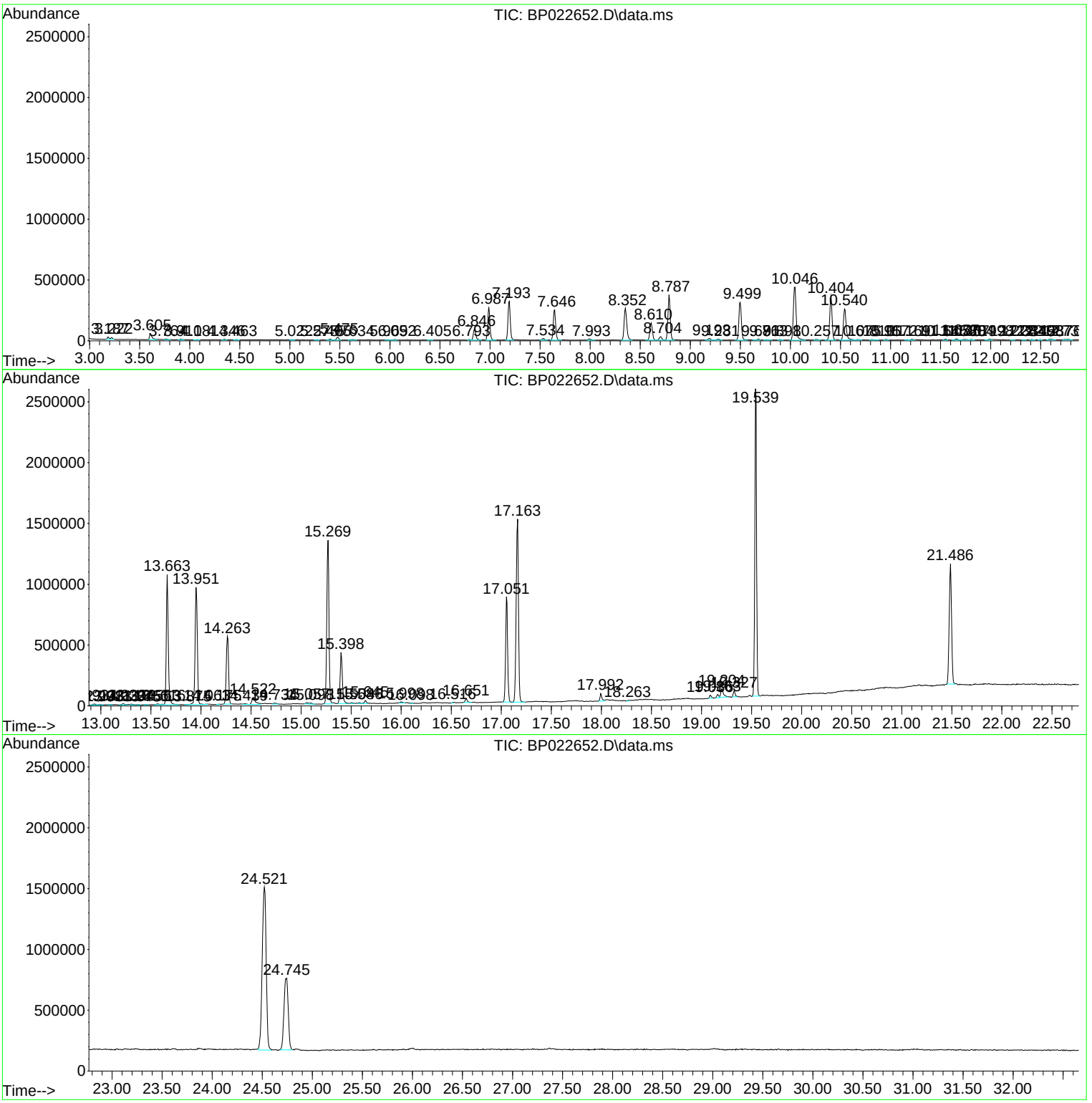
Acq On : 26 Oct 2024 21:24
Operator : RC/JU
Sample : P4559-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCNW6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.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\BP102524\
Data File : BP022652.D
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Operator : RC/JU
Sample : P4559-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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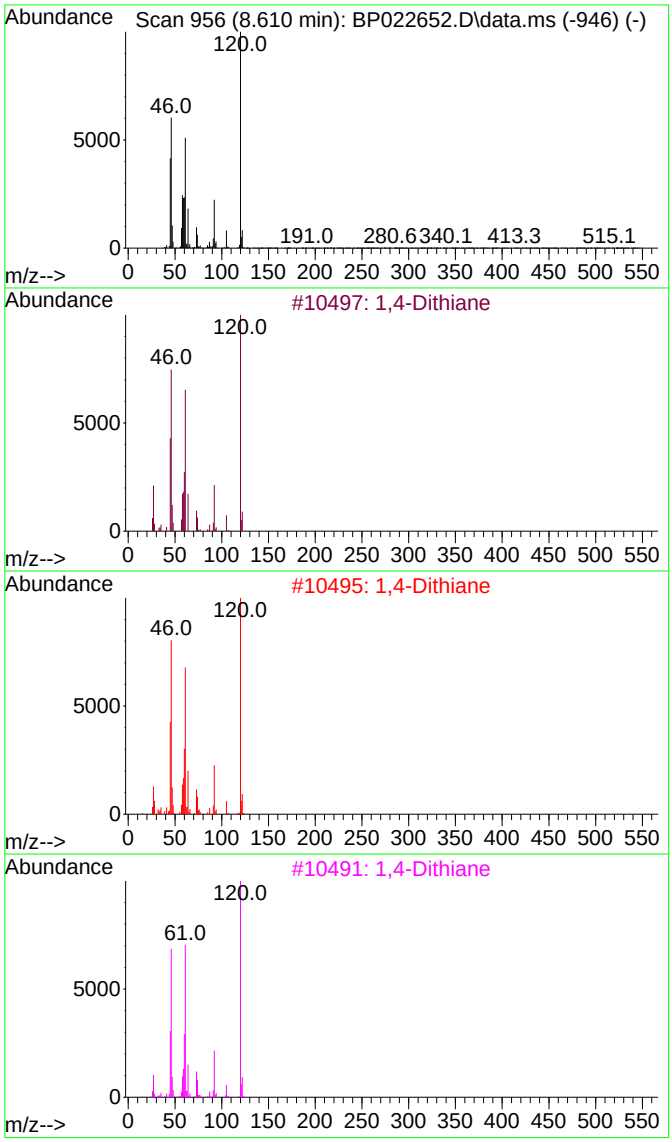
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
Quant Title : SVOA CALIBRATION

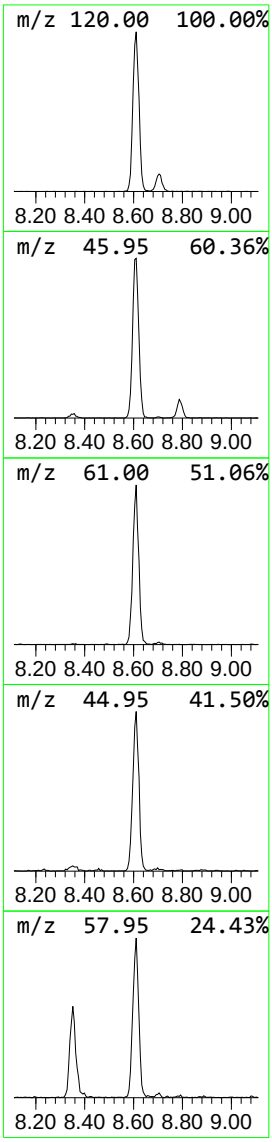
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 1,4-Dithiane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.610	12.06 ng/ul	249289	1,4-Dichlorobenzene-d4	7.646

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dithiane	120	C4H8S2	000505-29-3	97
2	1,4-Dithiane	120	C4H8S2	000505-29-3	96
3	1,4-Dithiane	120	C4H8S2	000505-29-3	93
4	1,4-Dithiane	120	C4H8S2	000505-29-3	91
5	1,3-Dithiane	120	C4H8S2	000505-23-7	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102524\
Data File : BP022652.D
Acq On : 26 Oct 2024 21:24
Operator : RC/JU
Sample : P4559-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCNW6

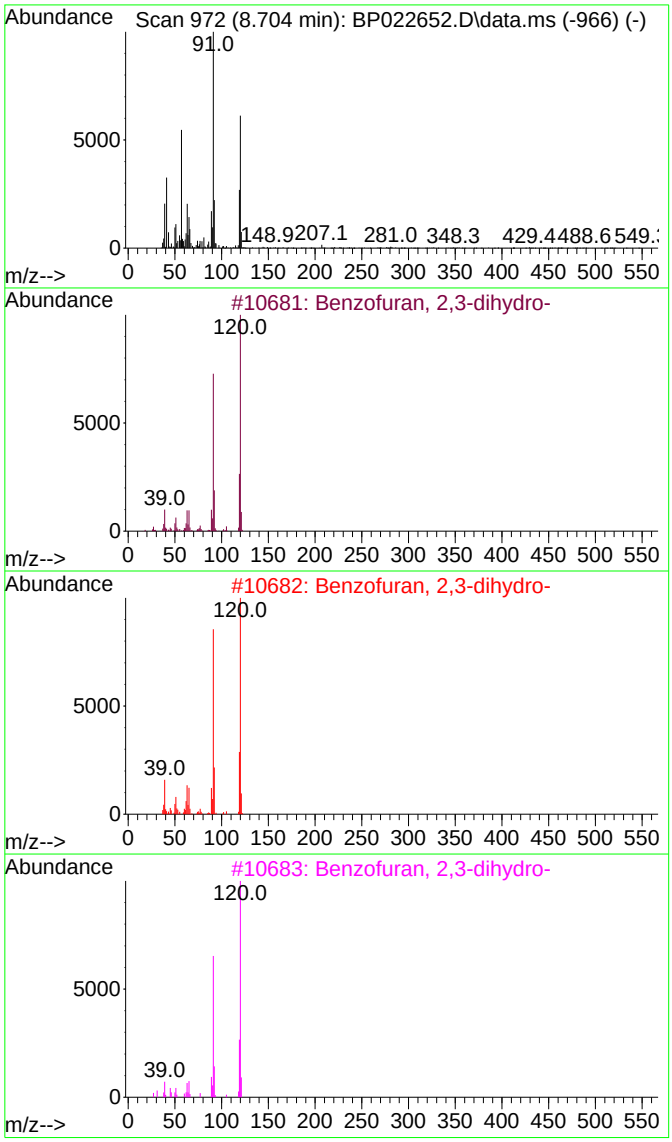
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
Quant Title : SVOA CALIBRATION

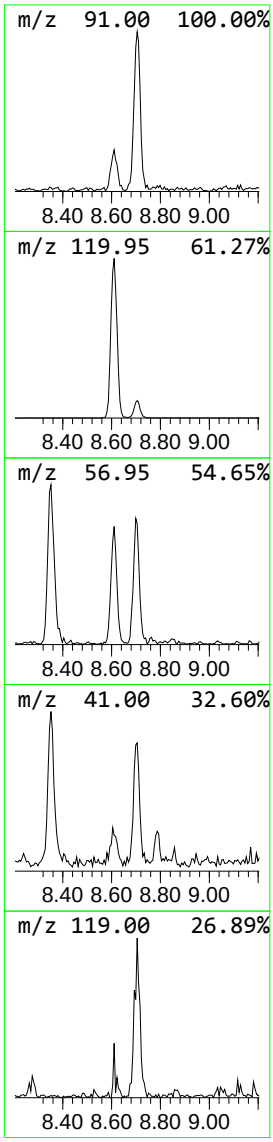
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzofuran, 2,3-dihydro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.704	2.27 ng/ul	46925	1,4-Dichlorobenzene-d4	7.646

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzofuran, 2,3-dihydro-	120	C8H8O	000496-16-2	90
2	Benzofuran, 2,3-dihydro-	120	C8H8O	000496-16-2	90
3	Benzofuran, 2,3-dihydro-	120	C8H8O	000496-16-2	74
4	Benzaldehyde, 3-methyl-	120	C8H8O	000620-23-5	62
5	Benzaldehyde, 4-methyl-	120	C8H8O	000104-87-0	62





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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCNW6

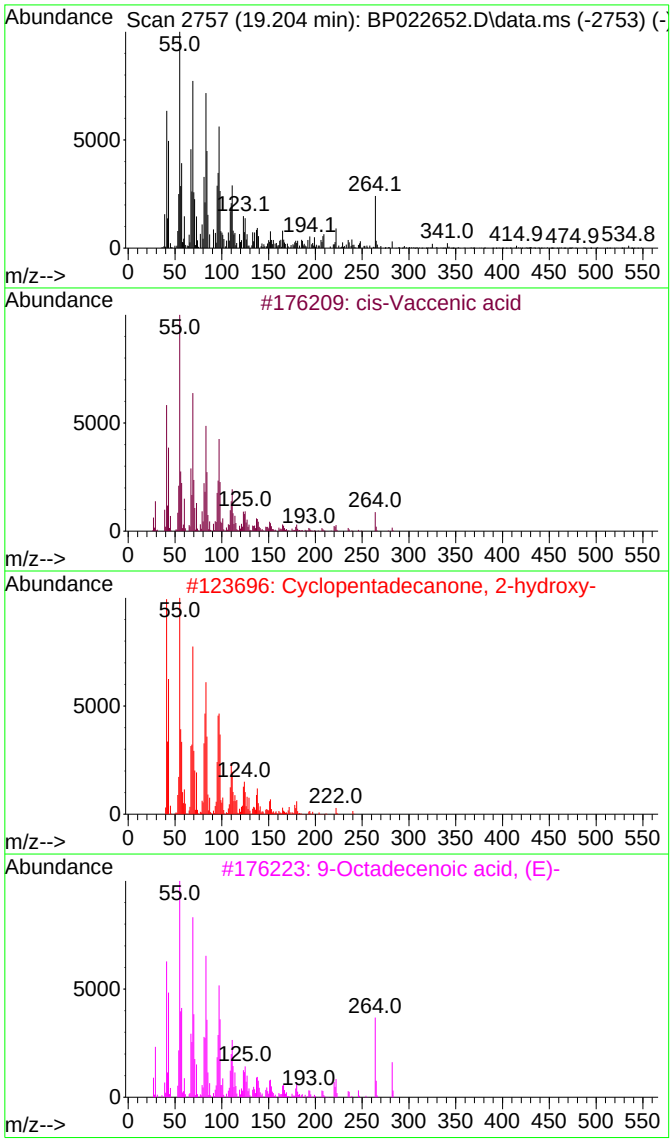
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
Quant Title : SVOA CALIBRATION

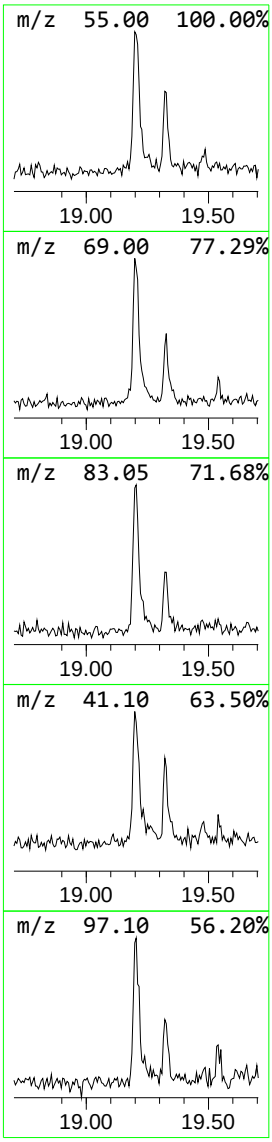
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 cis-Vaccenic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.204	2.20 ng/ul	132180	Phenanthrene-d10	17.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-Vaccenic acid	282	C18H34O2	000506-17-2	90
2	Cyclopentadecanone, 2-hydroxy-	240	C15H28O2	004727-18-8	86
3	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	80
4	n-Propyl 11-octadecenoate	324	C21H40O2	1000336-71-7	80
5	Oleic Acid	282	C18H34O2	000112-80-1	78





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102524\
Data File : BP022652.D
Acq On : 26 Oct 2024 21:24
Operator : RC/JU
Sample : P4559-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.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
1,4-Dithiane	8.610	12.1	ng/ul	249289	1	7.646	413513	20.0
Benzofuran, 2,3...	8.704	2.3	ng/ul	46925	1	7.646	413513	20.0
cis-Vaccenic acid	19.204	2.2	ng/ul	132180	4	17.051	1200520	20.0