LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112922\
Data File : BP012869.D
Acq On : 30 Nov 2022 00:53
Operator : CG/JU
Sample : N5725-04
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : BHB58

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: BP012869.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.393	31	35	39	rBV	118778	151233	1.01%	0.096%
2	3.428	39	41	49	rVB	42063	61399	0.41%	0.039%
3	3.823	106	108	120	rBV	446255	691279	4.59%	0.441%
4	4.058	143	148	154	rVB	55126	87707	0.58%	0.056%
5	4.158	161	165	168	rBV	44981	60137	0.40%	0.038%
6	6.487	557	561	567	rBV2	28950	48487	0.32%	0.031%
7	7.158	669	675	684	rBV	450358	702288	4.67%	0.448%
8	7.334	698	705	719	rBV	1878381	2925153	19.44%	1.865%
9	7.540	731	740	748	rBV	1218024	1959172	13.02%	1.249%
10	7.616	750	753	763	rVV9	15329	35652	0.24%	0.023%
11	8.011	813	820	827	rBV	2242173	3526578	23.44%	2.249%
12	8.387	878	884	889	rBV	78772	134270	0.89%	0.086%
13	8.558	908	913	918	rBV2	39070	61175	0.41%	0.039%
14	8.710	932	939	951	rBV	1181688	1873229	12.45%	1.194%
15	8.999	984	988	996	rVB6	14073	30747	0.20%	0.020%
16	9.093	998	1004	1011	rVV4	62063	128707	0.86%	0.082%
17	9.175	1011	1018	1031	rVV	2118151	3689346	24.52%	2.352%
18	9.287	1031	1037	1043	rVV4	30357	75031	0.50%	0.048%
19	9.375	1045	1052	1061	rVV	760571	1221959	8.12%	0.779%
20	9.487	1065	1071	1077	rVV	151959	284266	1.89%	0.181%
21	9.557	1077	1083	1095	rVB	429418	772841	5.14%	0.493%
22	9.899	1134	1141	1153	rBV	1190828	1968455	13.08%	1.255%
23	10.022	1158	1162	1166	rVV5	15432	29316	0.19%	0.019%
24	10.069	1166	1170	1174	rVV2	19354	37969	0.25%	0.024%
25	10.222	1191	1196	1205	rVB	80054	147257	0.98%	0.094%
26	10.440	1225	1233	1244	rBV	2081979	3392565	22.55%	2.163%
27	10.681	1268	1274	1278	rBV3	12795	29283	0.19%	0.019%
28	10.734	1278	1283	1287	rVV4	17791	31832	0.21%	0.020%
29	10.828	1287	1299	1305	rVV	3396890	5741942	38.16%	3.661%
30	10.881	1305	1308	1314	rVV2	78132	127582	0.85%	0.081%
31	10.957	1314	1321	1323	rVV	935449	1486110	9.88%	0.948%
32	10.999	1323	1328	1336	rVV	4806771	8472649	56.30%	5.402%
33	11.069	1336	1340	1344	rVV2	63162	106206	0.71%	0.068%
34	11.116	1344	1348	1355	rVV6	32904	65116	0.43%	0.042%
35	11.181	1355	1359	1364	rVV4	25152	49278	0.33%	0.031%
36	11.240	1364	1369	1375	rVB2	27891	49448	0.33%	0.032%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112922\
Data File : BP012869.D
Acq On : 30 Nov 2022 00:53
Operator : CG/JU
Sample : N5725-04
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BHB58

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	11.487	1404	1411	1419	rBV9	10951	32874	0.22%	0.021%
38	11.593	1425	1429	1435	rVB8	20217	30369	0.20%	0.019%
39	11.740	1449	1454	1458	rBV3	18365	28243	0.19%	0.018%
40	11.857	1466	1474	1481	rBV	28278	59629	0.40%	0.038%
41	11.940	1481	1488	1498	rBV	736946	1456702	9.68%	0.929%
42	12.087	1508	1513	1521	rVB8	20844	33988	0.23%	0.022%
43	12.334	1549	1555	1557	rBV6	19576	29190	0.19%	0.019%
44	12.375	1557	1562	1570	rVV2	182615	376787	2.50%	0.240%
45	12.440	1570	1573	1578	rVB2	34814	51004	0.34%	0.033%
46	12.675	1608	1613	1624	rBV2	63492	144978	0.96%	0.092%
47	12.887	1643	1649	1654	rBV	94166	157632	1.05%	0.101%
48	13.487	1744	1751	1755	rBV6	28010	61393	0.41%	0.039%
49	13.540	1755	1760	1765	rVB2	60524	110303	0.73%	0.070%
50	13.828	1804	1809	1816	rBV9	16749	31788	0.21%	0.020%
51	14.051	1840	1847	1858	rBV	5359195	7401967	49.19%	4.719%
52	14.340	1883	1896	1906	rBV	6641326	9787656	65.04%	6.241%
53	14.645	1941	1948	1955	rBV	5705343	8204303	54.52%	5.231%
54	14.710	1955	1959	1964	rVB	67721	101142	0.67%	0.064%
55	14.828	1973	1979	1998	rVB	336957	580759	3.86%	0.370%
56	15.045	2010	2016	2022	rVB	192161	295161	1.96%	0.188%
57	15.469	2084	2088	2096	rVB4	41220	90275	0.60%	0.058%
58	15.551	2096	2102	2103	rBV2	67001	99625	0.66%	0.064%
59	15.640	2110	2117	2123	rBV	9055271	12995182	86.36%	8.286%
60	15.698	2123	2127	2130	rVV2	58568	78610	0.52%	0.050%
61	15.745	2130	2135	2142	rVV	1785353	2338032	15.54%	1.491%
62	15.798	2142	2144	2148	rVB2	32413	43690	0.29%	0.028%
63	15.881	2155	2158	2165	rVB	41475	64171	0.43%	0.041%
64	15.992	2171	2177	2183	rBV3	184714	292977	1.95%	0.187%
65	16.134	2197	2201	2204	rBV4	49896	80519	0.54%	0.051%
66	16.363	2230	2240	2247	rBV	370393	748361	4.97%	0.477%
67	16.557	2266	2273	2277	rBV2	896058	1346008	8.94%	0.858%
68	16.604	2277	2281	2284	rVV2	89503	131158	0.87%	0.084%
69	16.675	2289	2293	2300	rVB	81806	132231	0.88%	0.084%
70	16.804	2309	2315	2321	rVB2	52497	103993	0.69%	0.066%
71	16.898	2322	2331	2334	rBV	674238	1280498	8.51%	0.816%
72	17.022	2347	2352	2358	rBV	214394	321346	2.14%	0.205%
73	17.116	2365	2368	2371	rBV2	23757	26512	0.18%	0.017%
74	17.157	2371	2375	2376	rVV3	39812	51376	0.34%	0.033%
75	17.204	2377	2383	2390	rVV	307559	570692	3.79%	0.364%
76	17.275	2390	2395	2406	rVV	278303	463296	3.08%	0.295%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112922\
Data File : BP012869.D
Acq On : 30 Nov 2022 00:53
Operator : CG/JU
Sample : N5725-04
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BHB58

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

77	17.398	2409	2416	2422	rVV	6587818	9682024	64.34%	6.173%
78	17.463	2422	2427	2428	rVV2	206748	351362	2.33%	0.224%
79	17.498	2428	2433	2443	rVV2	9546975	14348935	95.36%	9.149%
80	17.586	2445	2448	2451	rVV	85624	130565	0.87%	0.083%
81	17.622	2451	2454	2462	rVB	170817	274628	1.83%	0.175%
82	17.716	2467	2470	2473	rBV2	39537	49389	0.33%	0.031%
83	17.798	2482	2484	2493	rVB3	60945	127175	0.85%	0.081%
84	17.886	2496	2499	2505	rBV2	56918	95115	0.63%	0.061%
85	18.028	2520	2523	2525	rBV	36937	45449	0.30%	0.029%
86	18.057	2525	2528	2532	rVB	95660	106620	0.71%	0.068%
87	18.145	2539	2543	2548	rBV3	76060	131910	0.88%	0.084%
88	18.269	2560	2564	2572	rBV2	337477	469654	3.12%	0.299%
89	18.504	2601	2604	2609	rVB2	36851	49272	0.33%	0.031%
90	18.681	2631	2634	2639	rVB	80370	98385	0.65%	0.063%
91	19.122	2706	2709	2717	rVB2	88277	131776	0.88%	0.084%
92	19.304	2736	2740	2746	rBV3	121527	167262	1.11%	0.107%
93	19.369	2746	2751	2757	rBV2	149906	315975	2.10%	0.201%
94	19.498	2769	2773	2783	rBV3	155544	225549	1.50%	0.144%
95	19.645	2795	2798	2802	rVB	67924	74827	0.50%	0.048%
96	19.728	2806	2812	2825	rVV	11736243	15047898	100.00%	9.594%
97	21.175	3055	3058	3063	rBV2	253997	360846	2.40%	0.230%
98	21.486	3105	3111	3121	rBV	5752695	7889140	52.43%	5.030%
99	23.827	3502	3509	3525	rBV2	4441719	9497553	63.12%	6.056%
100	23.992	3530	3537	3552	rVB2	3204377	6678985	44.38%	4.258%

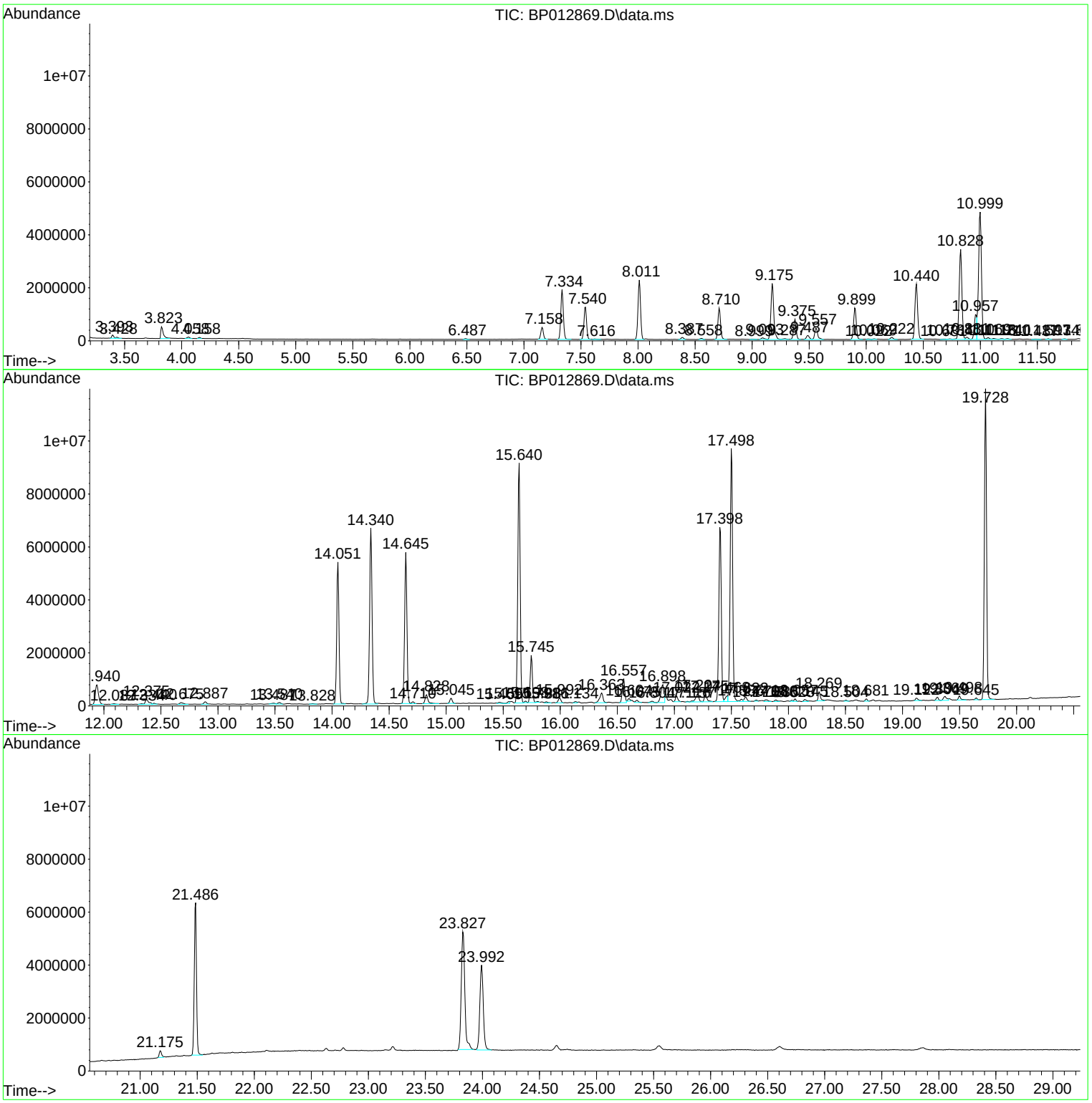
Sum of corrected areas: 156840378

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112922\
Data File : BP012869.D
Acq On : 30 Nov 2022 00:53
Operator : CG/JU
Sample : N5725-04
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BHB58

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\BP112922\
Data File : BP012869.D
Acq On : 30 Nov 2022 00:53
Operator : CG/JU
Sample : N5725-04
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BHB58

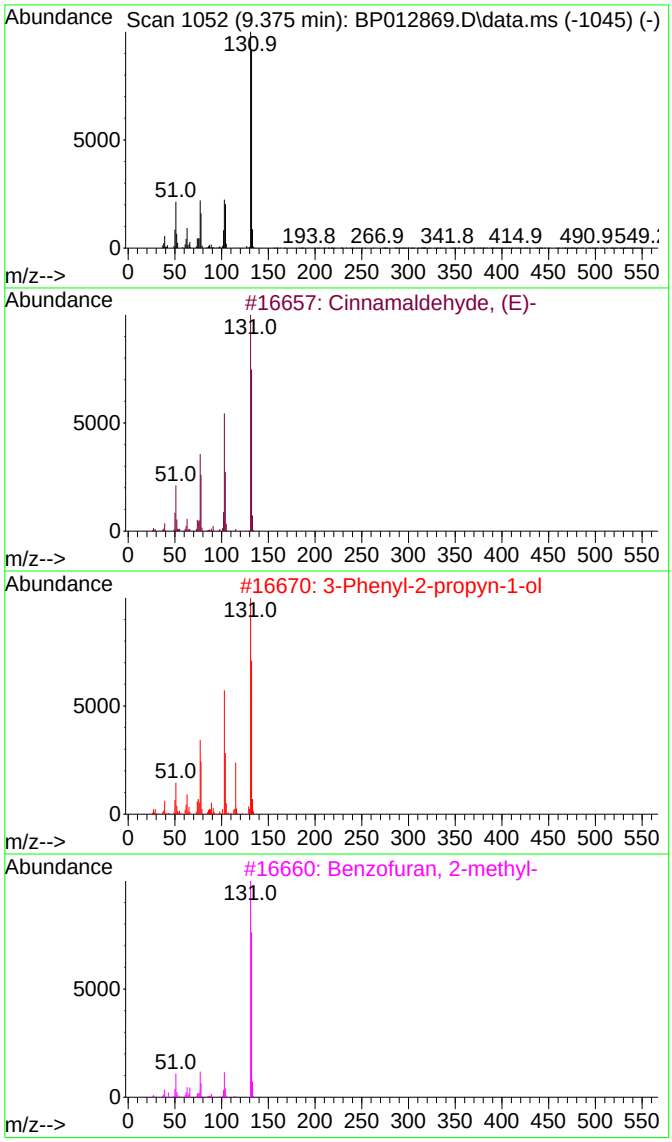
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP112522.M
Quant Title : SVOA CALIBRATION

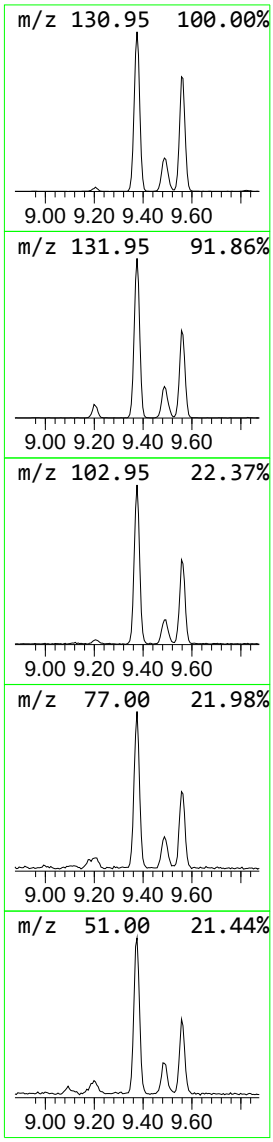
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Cinnamaldehyde, (E)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.375	6.93 ng/ul	1221960	1,4-Dichlorobenzene-d4	8.011

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamaldehyde, (E)-	132	C9H8O	014371-10-9	91
2	3-Phenyl-2-propyn-1-ol	132	C9H8O	001504-58-1	91
3	Benzofuran, 2-methyl-	132	C9H8O	004265-25-2	91
4	Benzofuran, 2-methyl-	132	C9H8O	004265-25-2	91
5	Benzofuran, 2-methyl-	132	C9H8O	004265-25-2	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112922\
Data File : BP012869.D
Acq On : 30 Nov 2022 00:53
Operator : CG/JU
Sample : N5725-04
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BHB58

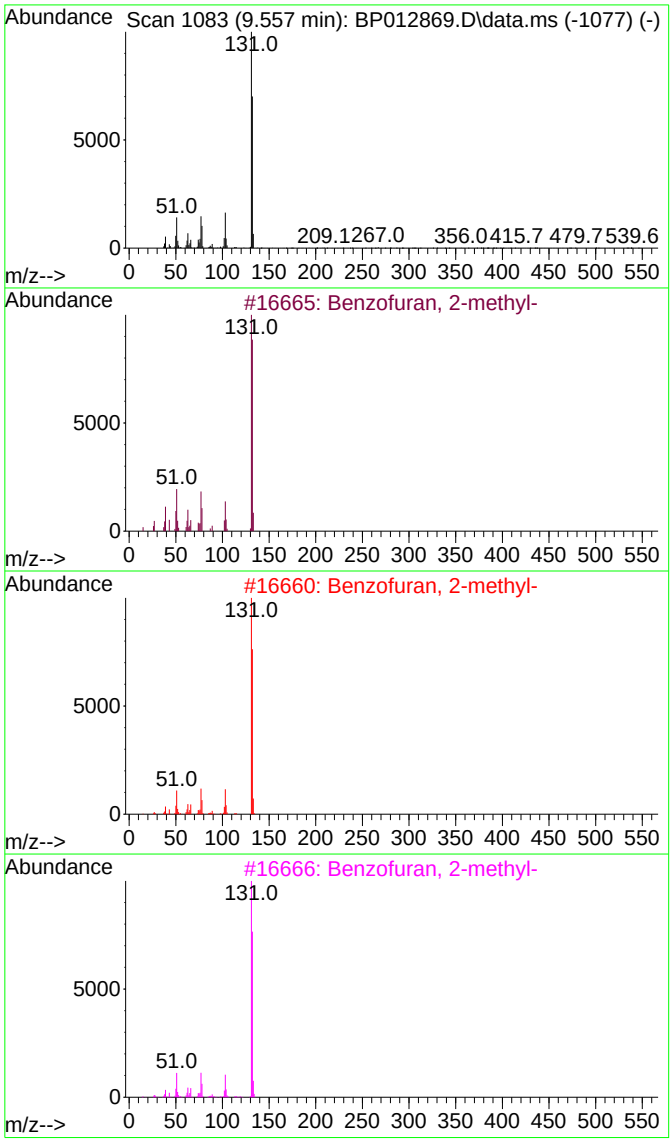
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP112522.M
Quant Title : SVOA CALIBRATION

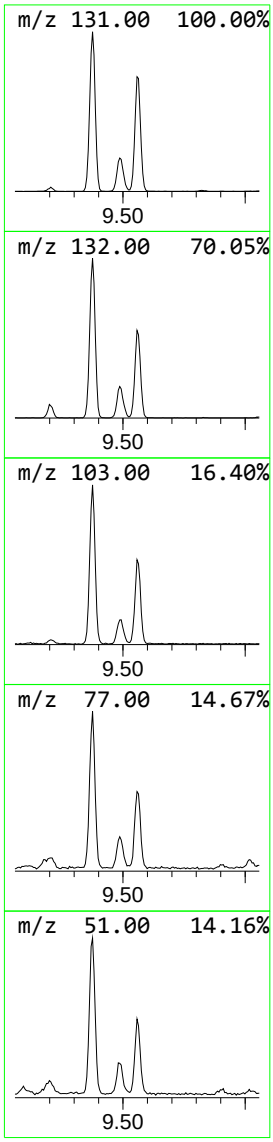
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzofuran, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.557	2.69 ng/ul	772841	Naphthalene-d8	10.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzofuran, 2-methyl-	132	C9H8O	004265-25-2	95
2	Benzofuran, 2-methyl-	132	C9H8O	004265-25-2	91
3	Benzofuran, 2-methyl-	132	C9H8O	004265-25-2	91
4	Benzofuran, 2-methyl-	132	C9H8O	004265-25-2	91
5	5-Methylbenzimidazole	132	C8H8N2	000614-97-1	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112922\
Data File : BP012869.D
Acq On : 30 Nov 2022 00:53
Operator : CG/JU
Sample : N5725-04
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BHB58

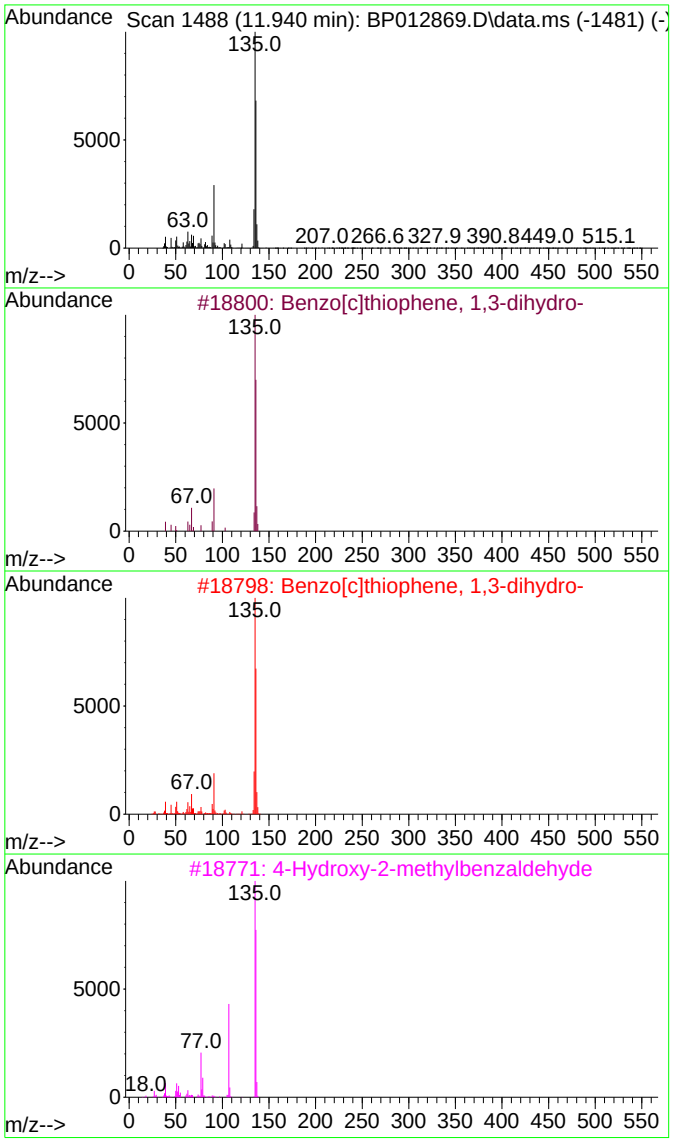
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP112522.M
Quant Title : SVOA CALIBRATION

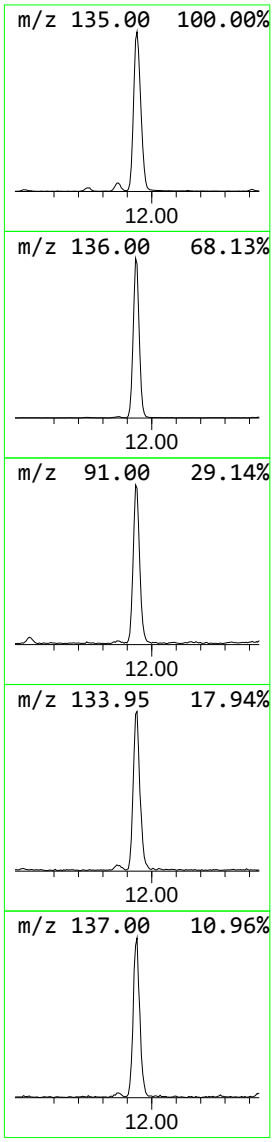
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzo[c]thiophene, 1,3-dihy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.940	5.07 ng/ul	1456700	Naphthalene-d8	10.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[c]thiophene, 1,3-dihydro-	136	C8H8S	002471-92-3	90
2	Benzo[c]thiophene, 1,3-dihydro-	136	C8H8S	002471-92-3	87
3	4-Hydroxy-2-methylbenzaldehyde	136	C8H8O2	041438-18-0	72
4	Benzene, (ethenylthio)-	136	C8H8S	001822-73-7	72
5	Pyrazine, 2,6-diethyl-	136	C8H12N2	013067-27-1	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112922\
Data File : BP012869.D
Acq On : 30 Nov 2022 00:53
Operator : CG/JU
Sample : N5725-04
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BHB58

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

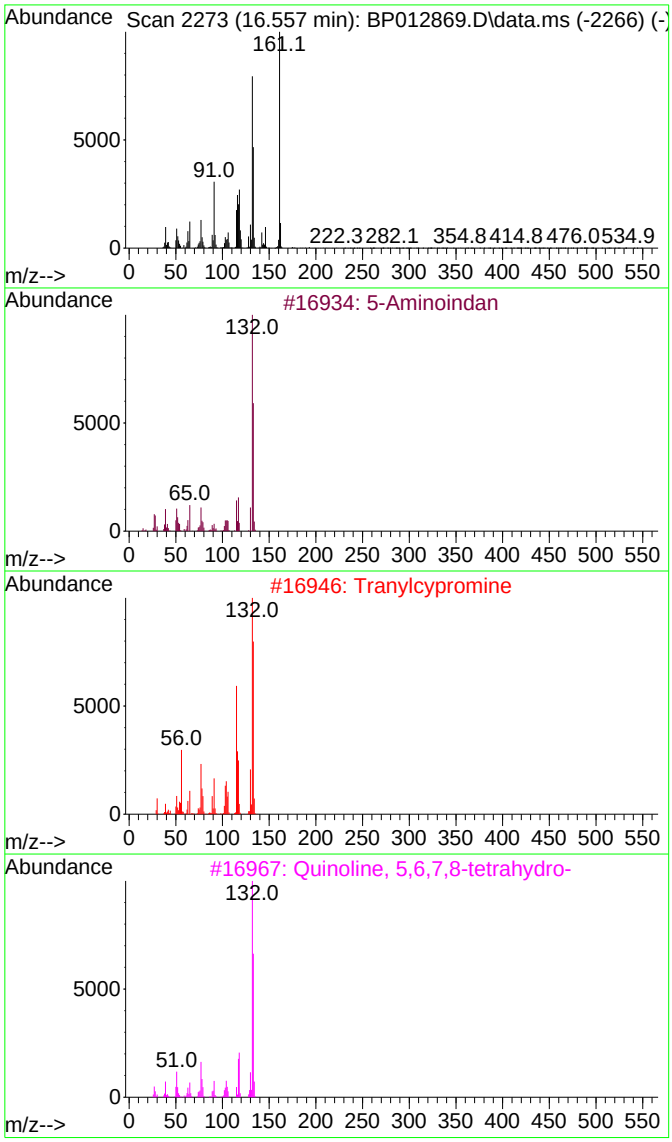
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

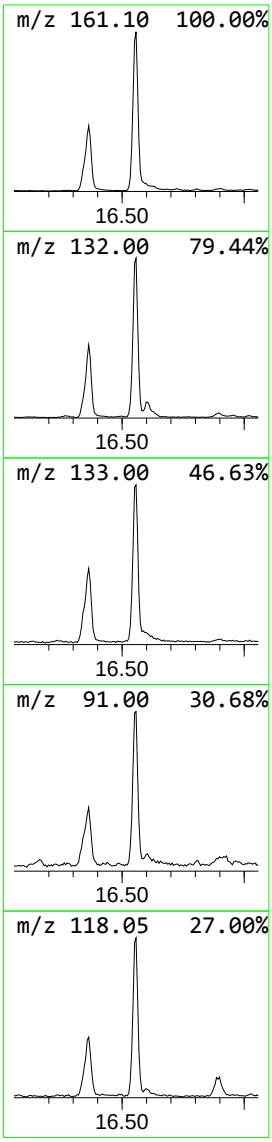
****

Peak Number 4 5-Aminoindan Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.557	2.78 ng/ul	1346010	Phenanthrene-d10	17.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindan	133	C9H11N	024425-40-9	86
2	Tranylcypromine	133	C9H11N	000155-09-9	55
3	Quinoline, 5,6,7,8-tetrahydro-	133	C9H11N	010500-57-9	49
4	Isoquinoline, 5,6,7,8-tetrahydro-	133	C9H11N	036556-06-6	46
5	1(2H)-naphthalenone, 5-amino-3,4...	161	C10H11NO	1000404-41-1	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112922\
Data File : BP012869.D
Acq On : 30 Nov 2022 00:53
Operator : CG/JU
Sample : N5725-04
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BHB58

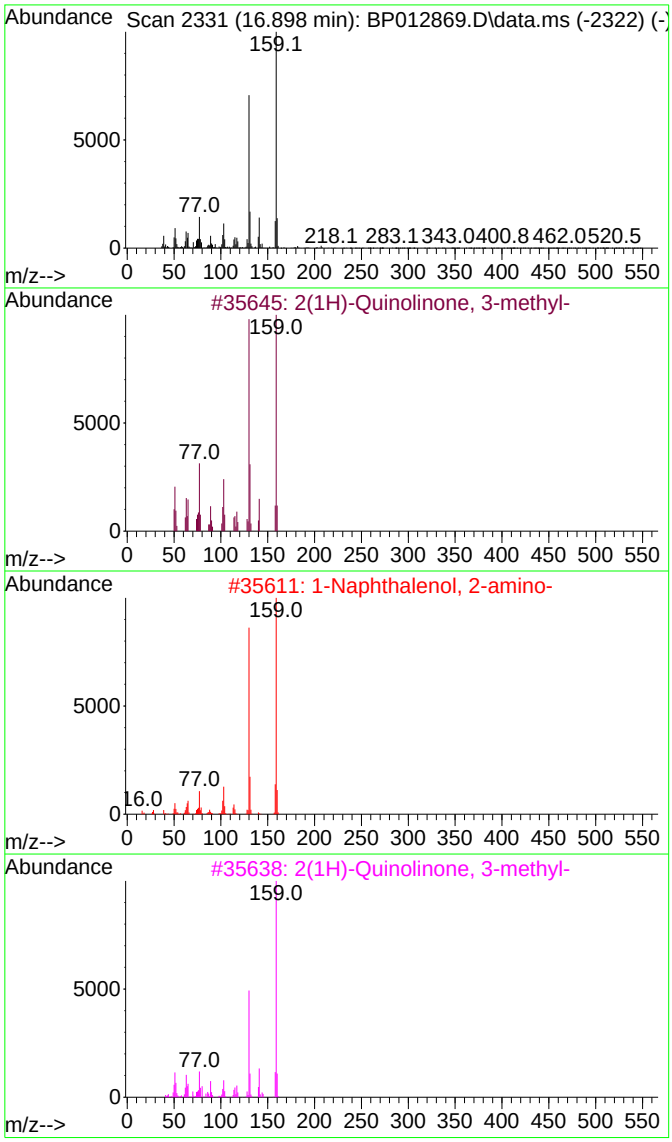
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP112522.M
Quant Title : SVOA CALIBRATION

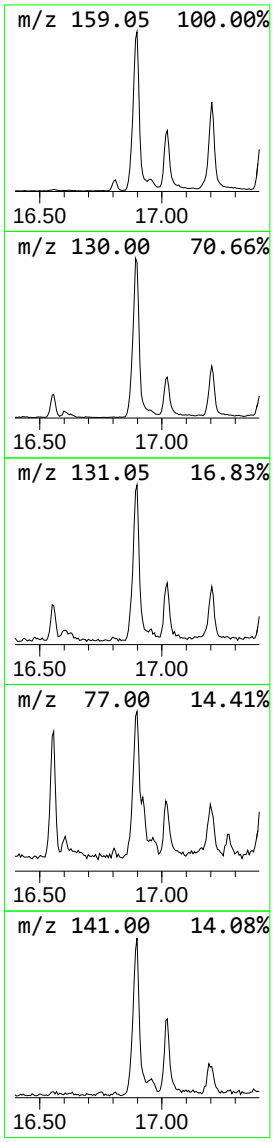
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2(1H)-Quinolinone, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.898	2.65 ng/ul	1280500	Phenanthrene-d10	17.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Quinolinone, 3-methyl-	159	C10H9NO	002721-59-7	97
2	1-Naphthalenol, 2-amino-	159	C10H9NO	000606-41-7	94
3	2(1H)-Quinolinone, 3-methyl-	159	C10H9NO	002721-59-7	93
4	1-Naphthalenol, 2-amino-	159	C10H9NO	000606-41-7	90
5	2-Naphthalenol, 1-amino-	159	C10H9NO	002834-92-6	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112922\
Data File : BP012869.D
Acq On : 30 Nov 2022 00:53
Operator : CG/JU
Sample : N5725-04
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BHB58

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
Cinnamaldehyde,...	9.375	6.9	ng/ul	1221960	1	8.011	3526580	20.0
Benzofuran, 2-m...	9.557	2.7	ng/ul	772841	2	10.828	5741940	20.0
Benzo[c]thiophe...	11.940	5.1	ng/ul	1456700	2	10.828	5741940	20.0
5-Aminoindan	16.557	2.8	ng/ul	1346010	4	17.398	9682020	20.0
2(1H)-Quinolino...	16.898	2.6	ng/ul	1280500	4	17.398	9682020	20.0