LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042624\
Data File : BN031250.D
Acq On : 26 Apr 2024 17:46
Operator : MA/JU
Sample : P2161-17
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0R89

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-BN041924.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BN031250.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.140	22	26	38	rVB	65727	90894	0.91%	0.092%
2	3.546	93	95	111	rBV	392948	602462	6.01%	0.608%
3	5.699	454	461	471	rBV2	37471	73422	0.73%	0.074%
4	6.634	615	620	627	rVB	18492	35994	0.36%	0.036%
5	6.799	642	648	660	rVV	335853	567560	5.66%	0.573%
6	6.969	670	677	695	rVB	1393498	2200518	21.94%	2.221%
7	7.158	700	709	720	rBV	1335753	2071633	20.65%	2.091%
8	7.622	781	788	794	rBV	1076965	1675103	16.70%	1.691%
9	7.687	794	799	810	rVB	235906	384380	3.83%	0.388%
10	7.869	825	830	834	rBV4	17471	33036	0.33%	0.033%
11	8.240	888	893	902	rVV	68098	127054	1.27%	0.128%
12	8.334	902	909	916	rVV	1010057	1665661	16.61%	1.681%
13	8.387	916	918	923	rVV4	15967	30581	0.30%	0.031%
14	8.446	924	928	938	rVB	33604	55778	0.56%	0.056%
15	8.716	965	974	979	rBV	581610	933181	9.30%	0.942%
16	8.781	979	985	991	rVV	1727261	2797769	27.89%	2.824%
17	8.828	991	993	999	rVV	50132	76861	0.77%	0.078%
18	9.169	1044	1051	1058	rBV2	39488	68466	0.68%	0.069%
19	9.493	1097	1106	1112	rBV	1399370	2312037	23.05%	2.334%
20	9.540	1112	1114	1119	rVB2	56575	70147	0.70%	0.071%
21	9.663	1128	1135	1141	rVB3	37460	85579	0.85%	0.086%
22	9.728	1141	1146	1157	rVB5	27092	56903	0.57%	0.057%
23	9.852	1157	1167	1171	rBV9	10698	28655	0.29%	0.029%
24	9.905	1171	1176	1184	rBV	88470	146616	1.46%	0.148%
25	10.028	1190	1197	1215	rVB	1954156	3297734	32.88%	3.329%
26	10.187	1217	1224	1228	rBV5	25087	52638	0.52%	0.053%
27	10.316	1240	1246	1254	rBV2	157684	263772	2.63%	0.266%
28	10.405	1254	1261	1267	rVV	1523508	2549920	25.42%	2.574%
29	10.463	1267	1271	1277	rVB	72041	112515	1.12%	0.114%
30	10.552	1277	1286	1297	rBV	1755229	3040636	30.31%	3.069%
31	10.775	1318	1324	1337	rVB	10548	32455	0.32%	0.033%
32	10.940	1345	1352	1358	rBV2	33661	59860	0.60%	0.060%
33	11.005	1358	1363	1367	rVV2	17616	30646	0.31%	0.031%
34	11.057	1367	1372	1382	rVB	52772	98024	0.98%	0.099%
35	11.193	1390	1395	1401	rVB2	31788	57369	0.57%	0.058%
36	11.305	1409	1414	1421	rBV	16490	29092	0.29%	0.029%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042624\
Data File : BN031250.D
Acq On : 26 Apr 2024 17:46
Operator : MA/JU
Sample : P2161-17
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0R89

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-BN041924.MA.M
Title : SVOA CALIBRATION

37	11.393	1424	1429	1436	rBV2	26642	52433	0.52%	0.053%
38	11.575	1451	1460	1464	rBV	40449	84387	0.84%	0.085%
39	11.610	1464	1466	1469	rVV3	22610	32661	0.33%	0.033%
40	11.657	1470	1474	1477	rVV3	23637	43582	0.43%	0.044%
41	11.699	1477	1481	1494	rVB	133001	248950	2.48%	0.251%
42	11.999	1521	1532	1539	rBV2	46240	100871	1.01%	0.102%
43	12.463	1604	1611	1616	rBV5	19811	38237	0.38%	0.039%
44	12.534	1619	1623	1630	rVV8	15202	37314	0.37%	0.038%
45	12.616	1630	1637	1643	rVV6	20167	55845	0.56%	0.056%
46	12.722	1651	1655	1667	rVB2	41891	84997	0.85%	0.086%
47	12.869	1674	1680	1684	rVB2	30426	42512	0.42%	0.043%
48	13.046	1703	1710	1718	rBV	95085	189603	1.89%	0.191%
49	13.116	1718	1722	1726	rVV	36083	56480	0.56%	0.057%
50	13.193	1726	1735	1751	rVB	972811	1565265	15.60%	1.580%
51	13.640	1806	1811	1813	rBV	25948	33322	0.33%	0.034%
52	13.693	1813	1820	1825	rVB	3932473	5596687	55.80%	5.649%
53	13.799	1833	1838	1844	rBV8	18290	31001	0.31%	0.031%
54	13.963	1856	1866	1872	rBV2	4400940	6672799	66.52%	6.736%
55	14.022	1872	1876	1881	rVV	78042	116707	1.16%	0.118%
56	14.140	1890	1896	1906	rVB	254728	387636	3.86%	0.391%
57	14.269	1910	1918	1926	rVB	2386985	3575078	35.64%	3.609%
58	14.357	1926	1933	1938	rBV4	19784	31421	0.31%	0.032%
59	14.487	1948	1955	1962	rBV	313156	518717	5.17%	0.524%
60	14.540	1962	1964	1971	rVB3	33310	49321	0.49%	0.050%
61	14.698	1986	1991	1997	rBV8	20241	46969	0.47%	0.047%
62	14.957	2028	2035	2042	rBV2	48469	87033	0.87%	0.088%
63	15.081	2051	2056	2068	rVB4	53571	152859	1.52%	0.154%
64	15.269	2081	2088	2098	rVB	5649418	8223268	81.98%	8.301%
65	15.393	2100	2109	2123	rBV	1311632	2028168	20.22%	2.047%
66	15.504	2124	2128	2134	rVB3	39515	59488	0.59%	0.060%
67	15.640	2147	2151	2162	rVB	77122	145894	1.45%	0.147%
68	15.840	2181	2185	2191	rBV8	17782	31498	0.31%	0.032%
69	15.993	2207	2211	2214	rVV	38412	57331	0.57%	0.058%
70	16.051	2218	2221	2226	rVV3	23927	36083	0.36%	0.036%
71	16.434	2282	2286	2292	rBV6	19299	32606	0.33%	0.033%
72	16.498	2292	2297	2302	rBV5	26303	43933	0.44%	0.044%
73	16.787	2341	2346	2351	rBV2	63317	90542	0.90%	0.091%
74	16.910	2361	2367	2371	rBV6	20540	42997	0.43%	0.043%
75	17.022	2379	2386	2395	rBV	2949973	4183769	41.71%	4.223%
76	17.122	2396	2403	2413	rVV2	6051998	8590497	85.64%	8.671%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042624\
Data File : BN031250.D
Acq On : 26 Apr 2024 17:46
Operator : MA/JU
Sample : P2161-17
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0R89

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-BN041924.MA.M
Title : SVOA CALIBRATION

77	17.316	2431	2436	2443	rVB	51795	74234	0.74%	0.075%
78	17.522	2464	2471	2480	rBV2	86200	131097	1.31%	0.132%
79	17.692	2493	2500	2514	rBV	1119911	1495916	14.91%	1.510%
80	17.922	2534	2539	2544	rBV	152749	224976	2.24%	0.227%
81	17.998	2549	2552	2554	rBV	38358	48034	0.48%	0.048%
82	18.134	2571	2575	2579	rBV	67885	93591	0.93%	0.094%
83	18.175	2579	2582	2585	rVB4	25864	34391	0.34%	0.035%
84	18.216	2585	2589	2592	rBV	87692	104970	1.05%	0.106%
85	18.257	2592	2596	2605	rVB2	73130	130036	1.30%	0.131%
86	18.422	2619	2624	2627	rBV6	16819	31085	0.31%	0.031%
87	18.857	2694	2698	2702	rBV	82372	97114	0.97%	0.098%
88	18.986	2715	2720	2724	rBV	105853	146597	1.46%	0.148%
89	19.057	2728	2732	2735	rBV	105155	142590	1.42%	0.144%
90	19.210	2754	2758	2765	rBV2	113936	174169	1.74%	0.176%
91	19.363	2781	2784	2787	rVB	39231	44916	0.45%	0.045%
92	19.428	2788	2795	2801	rBV2	7136819	10030628	100.00%	10.125%
93	19.822	2860	2862	2869	rVB4	39271	50703	0.51%	0.051%
94	19.981	2886	2889	2892	rVB	46008	48426	0.48%	0.049%
95	20.439	2960	2967	2971	rBV4	162529	301834	3.01%	0.305%
96	21.257	3100	3106	3117	rBV	2779623	3909550	38.98%	3.946%
97	22.610	3332	3336	3343	rVB3	117051	206924	2.06%	0.209%
98	23.327	3454	3458	3465	rVB3	120458	227088	2.26%	0.229%
99	23.957	3556	3565	3579	rVB	3294869	8171392	81.46%	8.248%
100	24.157	3590	3599	3612	rVB	1553136	3832091	38.20%	3.868%

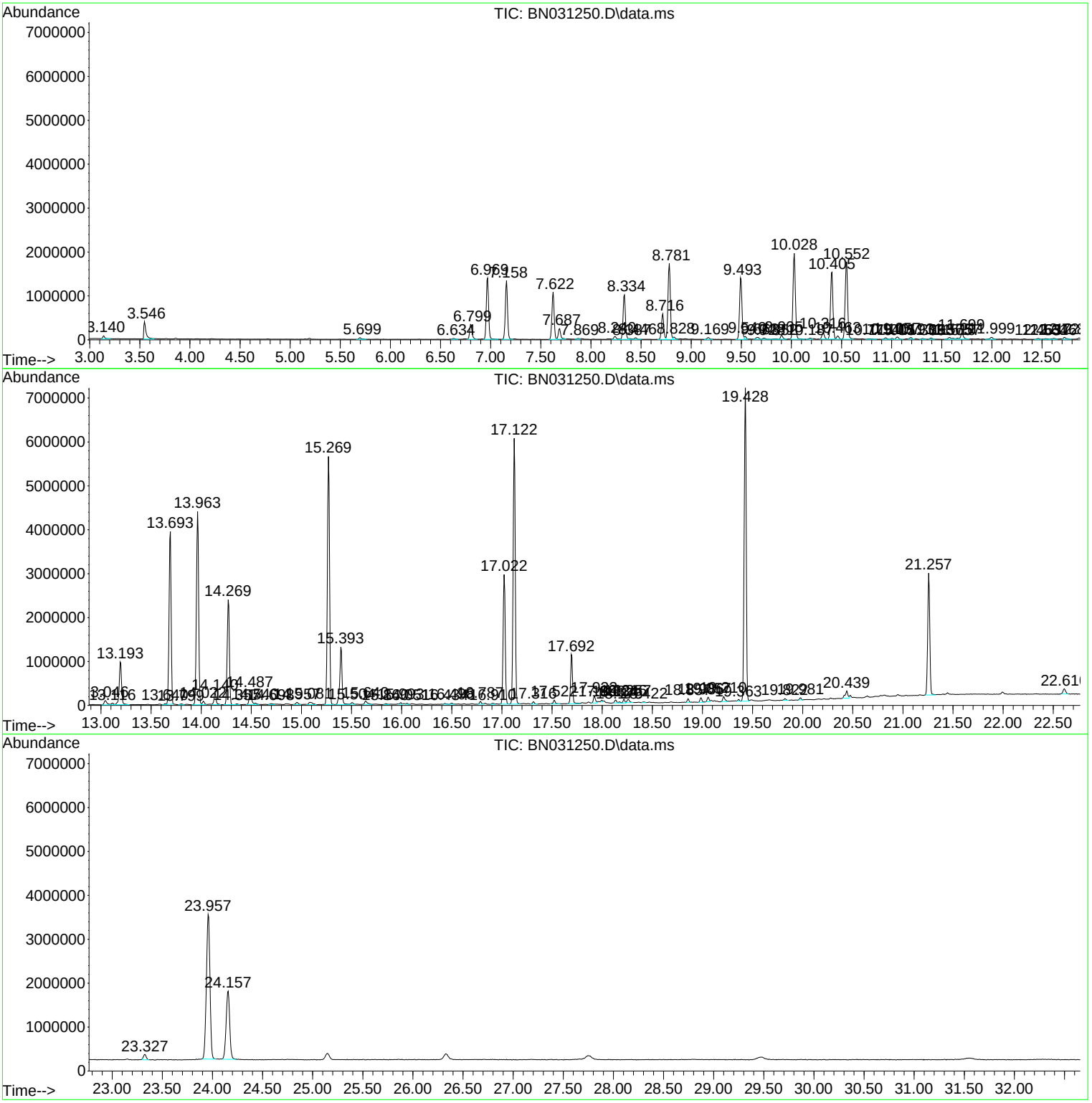
Sum of corrected areas: 99066064

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042624\
Data File : BN031250.D
Acq On : 26 Apr 2024 17:46
Operator : MA/JU
Sample : P2161-17
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0R89

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041924.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\BN042624\
Data File : BN031250.D
Acq On : 26 Apr 2024 17:46
Operator : MA/JU
Sample : P2161-17
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0R89

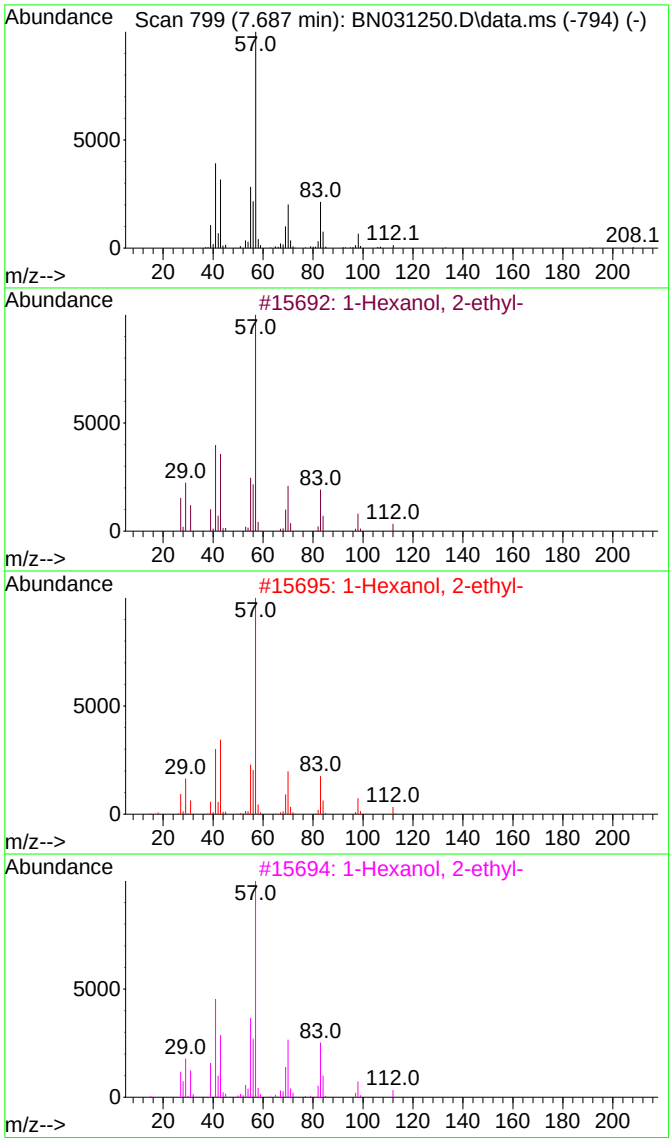
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041924.MA.M
Quant Title : SVOA CALIBRATION

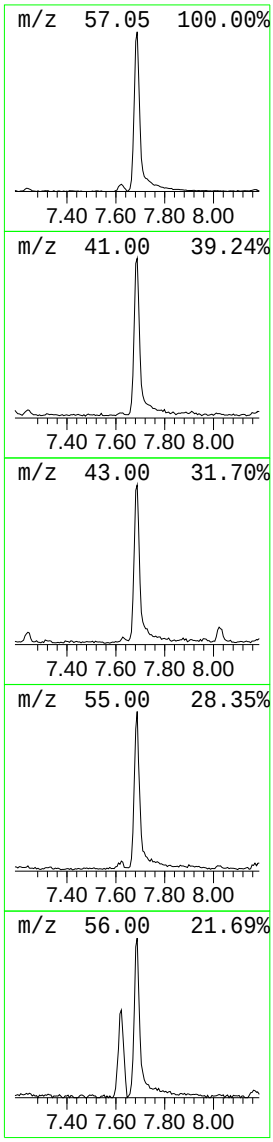
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.687	4.59 ng/ul	384380	1,4-Dichlorobenzene-d4	7.622

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	56
5	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042624\
Data File : BN031250.D
Acq On : 26 Apr 2024 17:46
Operator : MA/JU
Sample : P2161-17
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0R89

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041924.MA.M
Quant Title : SVOA CALIBRATION

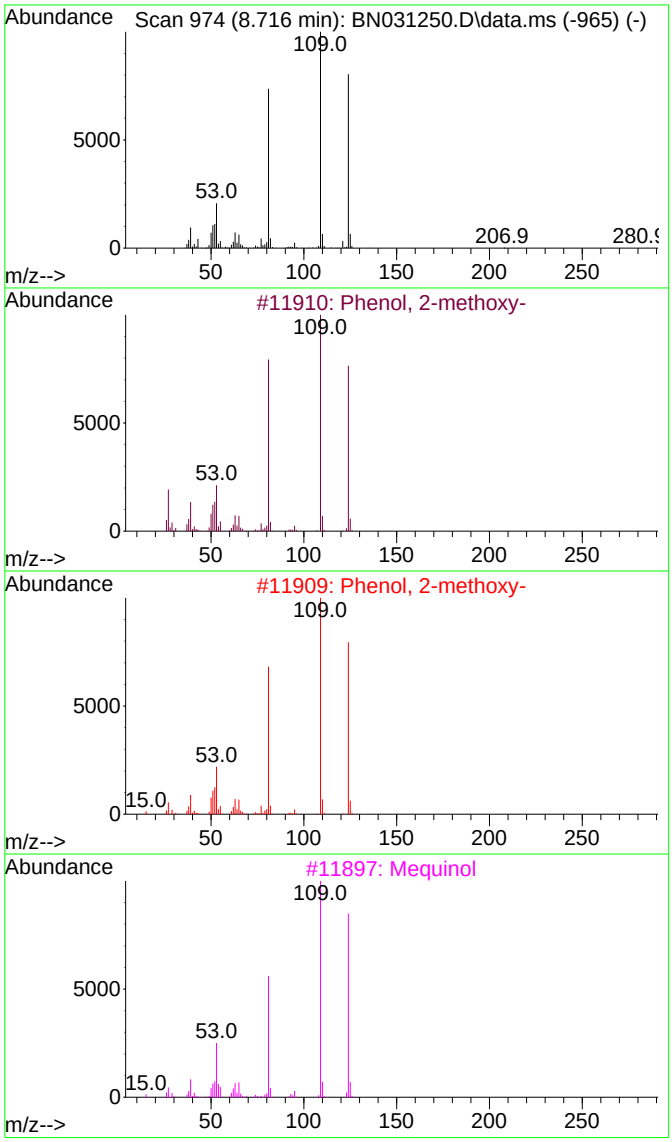
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

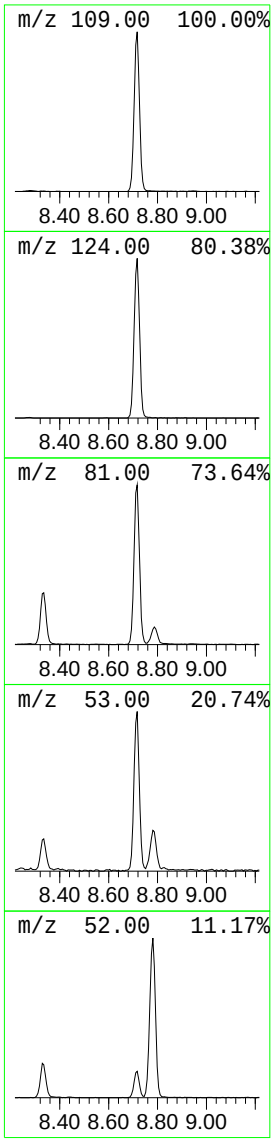
****

Peak Number 2 Phenol, 2-methoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.716	11.14 ng/ul	933181	1,4-Dichlorobenzene-d4	7.622

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	97
2	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	96
3	Mequinol	124	C7H8O2	000150-76-5	91
4	Mequinol	124	C7H8O2	000150-76-5	90
5	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042624\
Data File : BN031250.D
Acq On : 26 Apr 2024 17:46
Operator : MA/JU
Sample : P2161-17
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0R89

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041924.MA.M
Quant Title : SVOA CALIBRATION

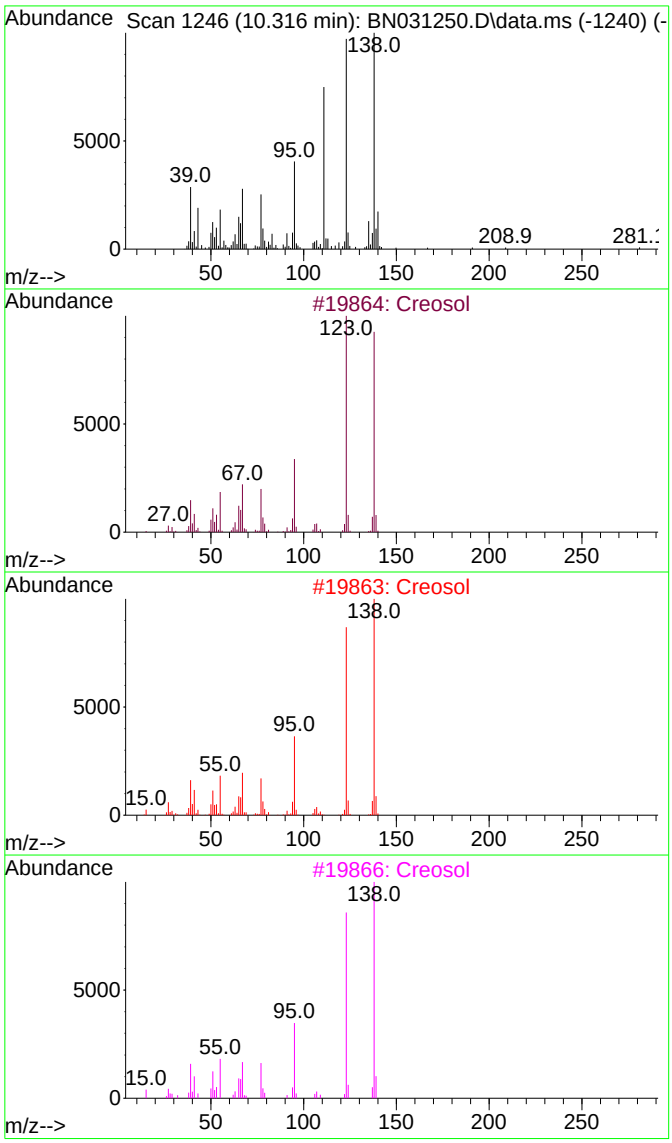
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

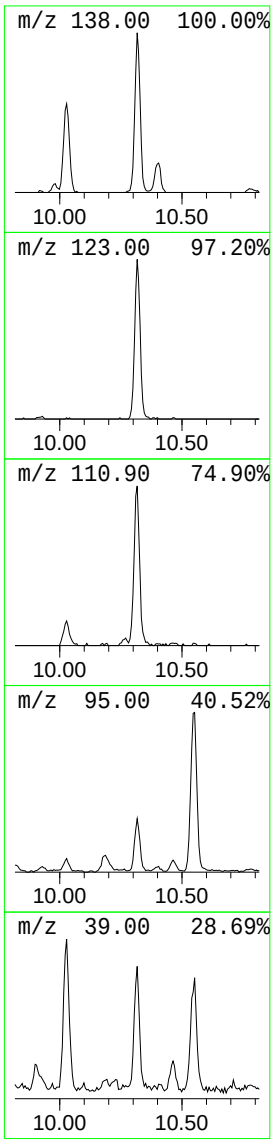
****

Peak Number 3 Creosol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.316	2.07 ng/ul	263772	Naphthalene-d8	10.405

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Creosol	138	C8H10O2	000093-51-6	98
2	Creosol	138	C8H10O2	000093-51-6	96
3	Creosol	138	C8H10O2	000093-51-6	93
4	2-Methoxy-5-methylphenol	138	C8H10O2	001195-09-1	92
5	Creosol	138	C8H10O2	000093-51-6	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042624\
Data File : BN031250.D
Acq On : 26 Apr 2024 17:46
Operator : MA/JU
Sample : P2161-17
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0R89

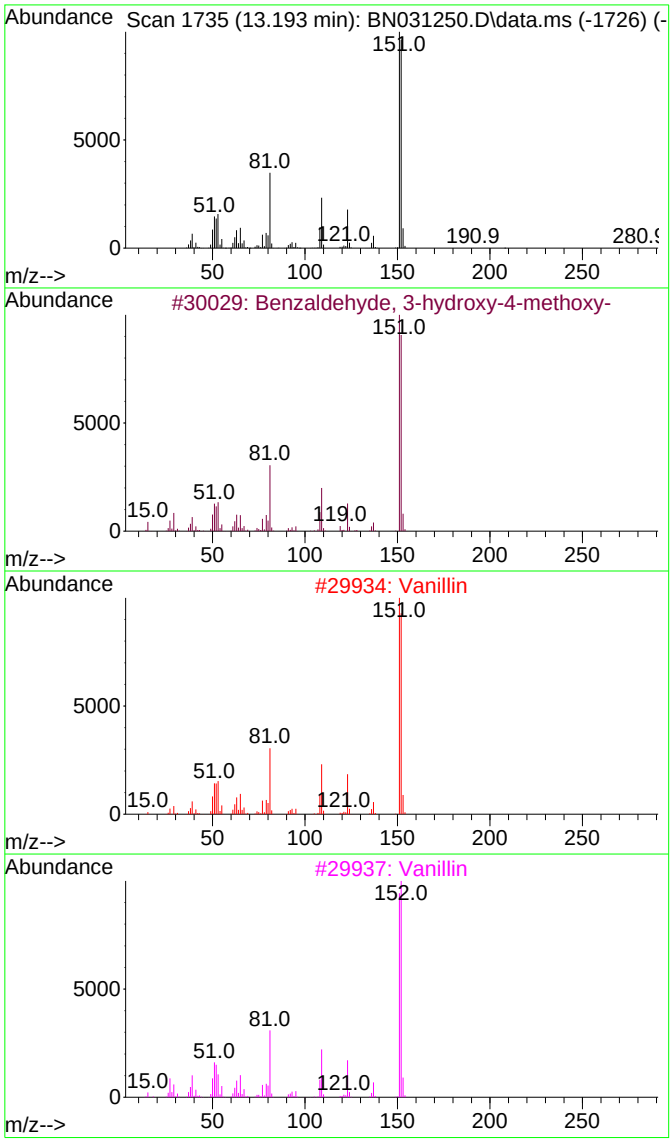
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041924.MA.M
Quant Title : SVOA CALIBRATION

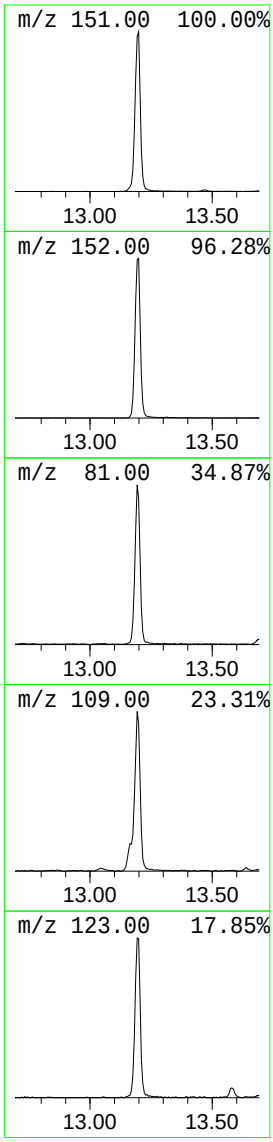
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzaldehyde, 3-hydroxy-4-m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.193	8.76 ng/ul	1565270	Acenaphthene-d10	14.269

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





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042624\
Data File : BN031250.D
Acq On : 26 Apr 2024 17:46
Operator : MA/JU
Sample : P2161-17
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0R89

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041924.MA.M
Quant Title : SVOA CALIBRATION

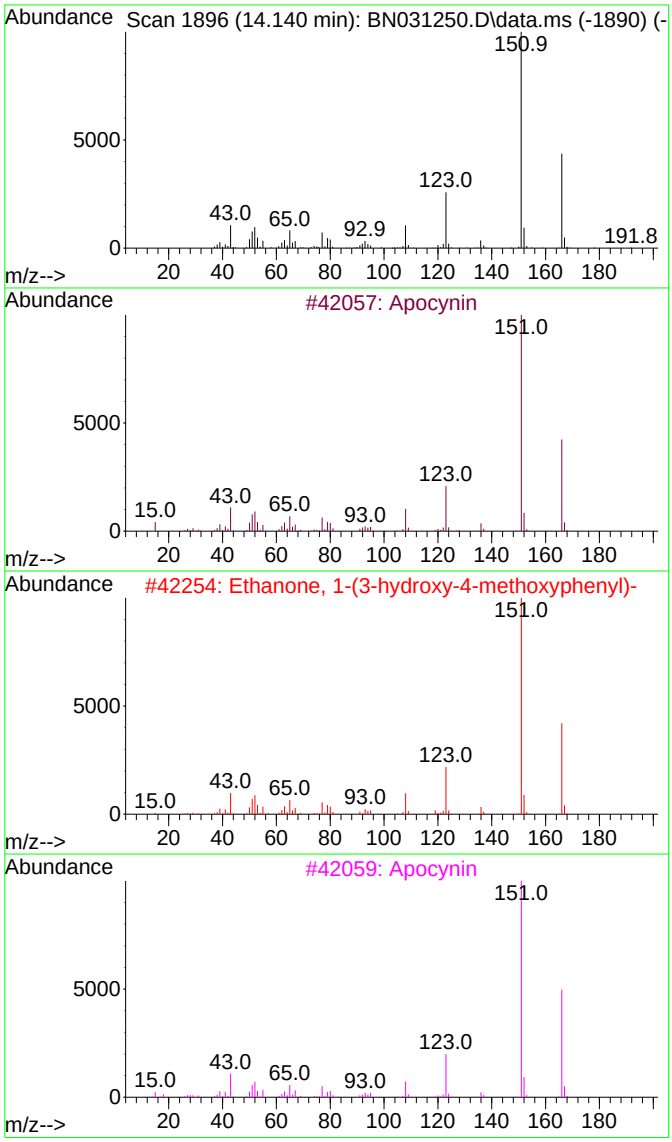
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

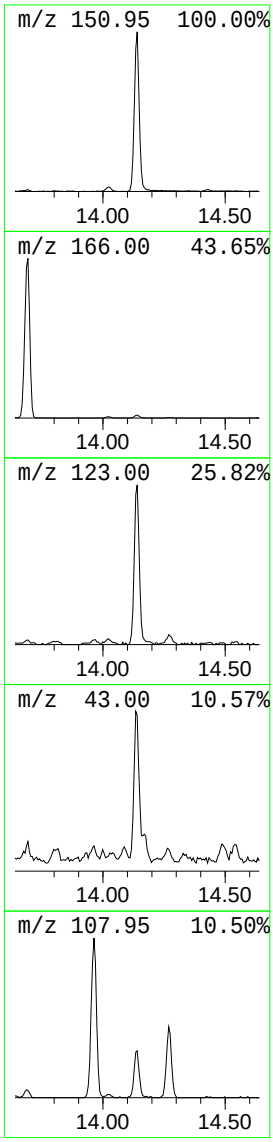
****

Peak Number 5 Apocynin Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.140	2.17 ng/ul	387636	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Apocynin	166	C9H10O3	000498-02-2	94
2	Ethanone, 1-(3-hydroxy-4-methoxy...	166	C9H10O3	006100-74-9	94
3	Apocynin	166	C9H10O3	000498-02-2	93
4	Apocynin	166	C9H10O3	000498-02-2	93
5	Ethanone, 1-(3-hydroxy-4-methoxy...	166	C9H10O3	006100-74-9	91





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Data File : BN031250.D
Acq On : 26 Apr 2024 17:46
Operator : MA/JU
Sample : P2161-17
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0R89

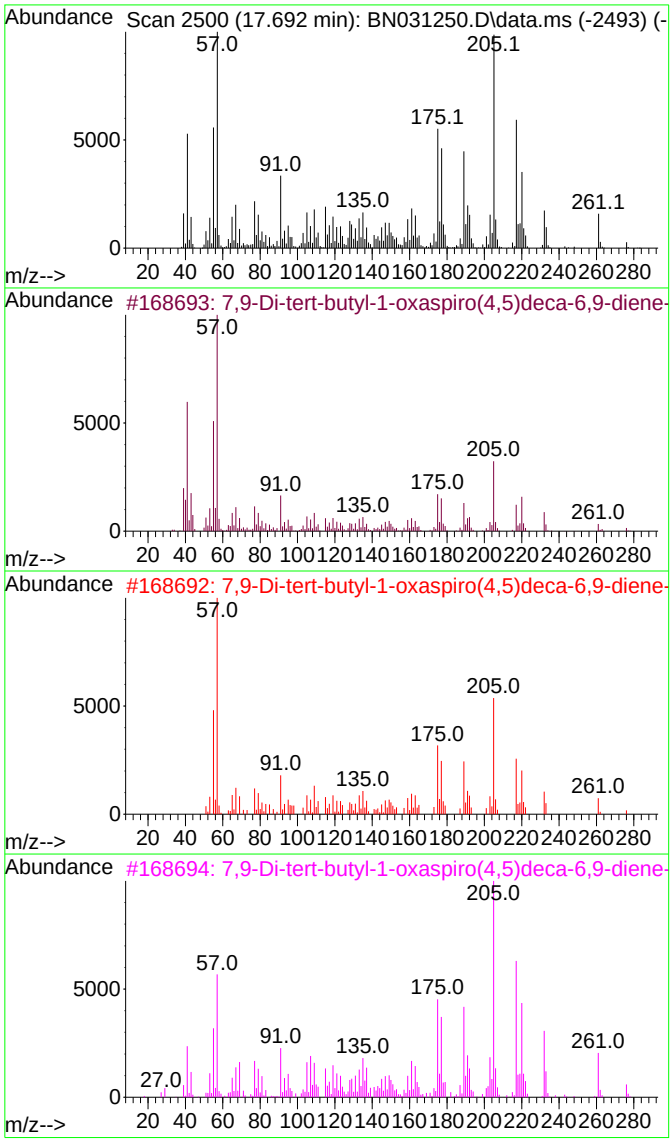
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041924.MA.M
Quant Title : SVOA CALIBRATION

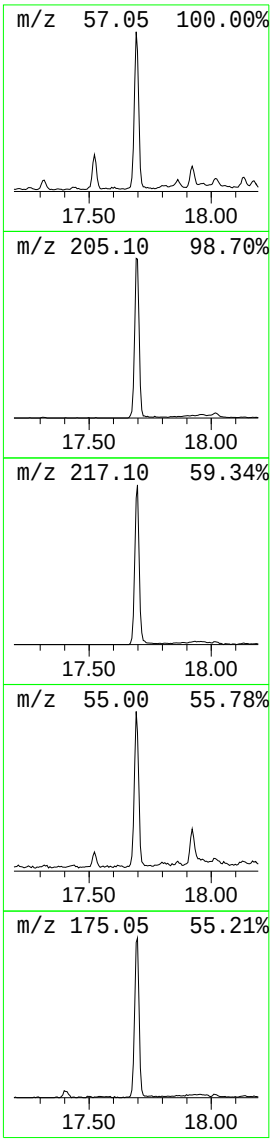
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.692	7.15 ng/ul	1495920	Phenanthrene-d10	17.022

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	99
3	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	94
4	2,5-Cyclohexadien-1-one, 2,6-bis...	232	C16H24O	006738-27-8	83
5	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042624\
Data File : BN031250.D
Acq On : 26 Apr 2024 17:46
Operator : MA/JU
Sample : P2161-17
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0R89

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041924.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...	7.687	4.6	ng/ul	384380	1	7.622	1675100	20.0
Phenol, 2-methoxy-	8.716	11.1	ng/ul	933181	1	7.622	1675100	20.0
Creosol	10.316	2.1	ng/ul	263772	2	10.405	2549920	20.0
Benzaldehyde, 3...	13.193	8.8	ng/ul	1565270	3	14.269	3575080	20.0
Apocynin	14.140	2.2	ng/ul	387636	3	14.269	3575080	20.0
7,9-Di-tert-but...	17.692	7.2	ng/ul	1495920	4	17.022	4183770	20.0