LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN111423\
Data File : BN028617.D
Acq On : 15 Nov 2023 00:20
Operator : MA/JU
Sample : 05337-18
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : GCDK4

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-BN111423.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BN028617.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.146	7	10	28	rVB2	64310	155221	2.18%	0.281%
2	3.581	81	84	89	rBV4	25333	47485	0.67%	0.086%
3	6.911	641	650	651	rBV8	31691	63449	0.89%	0.115%
4	7.046	667	673	698	rBV	235970	750793	10.57%	1.360%
5	7.234	698	705	731	rVV	364926	993902	13.99%	1.800%
6	7.705	779	785	809	rBV	229076	730390	10.28%	1.323%
7	8.428	901	908	928	rBV3	136244	632741	8.90%	1.146%
8	8.863	975	982	1009	rBV	358727	1187683	16.71%	2.151%
9	9.287	1052	1054	1060	rVB4	12299	17976	0.25%	0.033%
10	9.581	1096	1104	1125	rBV	290524	883378	12.43%	1.600%
11	10.122	1189	1196	1215	rBV	387406	1236707	17.40%	2.240%
12	10.387	1239	1241	1249	rVB9	11205	23795	0.33%	0.043%
13	10.487	1251	1258	1275	rBV	575510	1268723	17.85%	2.298%
14	10.646	1279	1285	1302	rBV	252344	959857	13.51%	1.739%
15	10.928	1327	1333	1343	rVB8	36157	97435	1.37%	0.177%
16	11.069	1353	1357	1365	rVB9	19152	46477	0.65%	0.084%
17	11.269	1387	1391	1393	rVB5	6880	8952	0.13%	0.016%
18	11.316	1393	1399	1400	rBV2	32528	47623	0.67%	0.086%
19	11.340	1400	1403	1411	rVV3	44167	84991	1.20%	0.154%
20	11.416	1411	1416	1419	rVV3	18119	27380	0.39%	0.050%
21	11.457	1419	1423	1428	rVB2	15927	25110	0.35%	0.045%
22	11.710	1464	1466	1471	rVB6	6494	9437	0.13%	0.017%
23	11.787	1474	1479	1486	rVB5	14050	25639	0.36%	0.046%
24	12.728	1634	1639	1649	rVB2	13400	33143	0.47%	0.060%
25	13.198	1713	1719	1722	rBV4	8458	13217	0.19%	0.024%
26	13.251	1722	1728	1737	rVV	191486	313187	4.41%	0.567%
27	13.763	1790	1815	1825	rBV	2401734	5429739	76.41%	9.836%
28	14.034	1854	1861	1885	rVB	2257551	3688054	51.90%	6.681%
29	14.340	1906	1913	1925	rBV	1118326	1851820	26.06%	3.355%
30	15.163	2047	2053	2059	rBV7	18349	31475	0.44%	0.057%
31	15.340	2077	2083	2099	rBV	2834203	4812471	67.72%	8.718%
32	15.463	2099	2104	2120	rVB	664301	1269552	17.87%	2.300%
33	15.792	2155	2160	2163	rBV2	35102	53870	0.76%	0.098%
34	15.910	2178	2180	2186	rVB7	7437	10685	0.15%	0.019%
35	16.092	2207	2211	2216	rBV	73345	95511	1.34%	0.173%
36	16.187	2222	2227	2231	rBV	133582	187923	2.64%	0.340%

LSC Area Percent Report

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Instrument :
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GCDK4

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-BN111423.MA.M
Title : SVOA CALIBRATION

37	16.245	2232	2237	2243	rVB2	192057	342087	4.81%	0.620%
38	16.304	2243	2247	2251	rBV2	153423	213459	3.00%	0.387%
39	16.345	2251	2254	2259	rVB	98319	125940	1.77%	0.228%
40	16.404	2259	2264	2265	rBV	47189	63024	0.89%	0.114%
41	16.451	2270	2272	2276	rVB	57241	59632	0.84%	0.108%
42	16.504	2276	2281	2288	rVB4	130411	256695	3.61%	0.465%
43	16.575	2288	2293	2296	rBV	132382	190377	2.68%	0.345%
44	16.645	2302	2305	2314	rVB	77872	112284	1.58%	0.203%
45	16.781	2325	2328	2333	rVB6	10157	14224	0.20%	0.026%
46	16.975	2357	2361	2366	rBV6	10767	17552	0.25%	0.032%
47	17.092	2375	2381	2392	rBV	1197354	1999093	28.13%	3.621%
48	17.192	2392	2398	2429	rVB	3406027	5730994	80.65%	10.382%
49	17.769	2493	2496	2503	rBV9	19832	32848	0.46%	0.060%
50	18.016	2534	2538	2546	rBV8	30805	76549	1.08%	0.139%
51	18.075	2546	2548	2554	rVB	15300	22196	0.31%	0.040%
52	18.222	2569	2573	2579	rBV3	33850	63076	0.89%	0.114%
53	18.510	2620	2622	2627	rBV6	10414	14771	0.21%	0.027%
54	18.775	2664	2667	2672	rBV	46639	53191	0.75%	0.096%
55	18.969	2697	2700	2704	rVB3	26123	29938	0.42%	0.054%
56	19.063	2712	2716	2721	rBV	45793	62915	0.89%	0.114%
57	19.133	2725	2728	2735	rVV	30472	47741	0.67%	0.086%
58	19.492	2784	2789	2815	rBV	4778109	7106293	100.00%	12.873%
59	21.304	3092	3097	3113	rBV	1254960	2260479	31.81%	4.095%
60	23.451	3456	3462	3471	rBV2	3660005	6915676	97.32%	12.528%
61	23.598	3482	3487	3498	rVB	1126169	2276715	32.04%	4.124%

Sum of corrected areas: 55203540

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Instrument :
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ClientSampleId :
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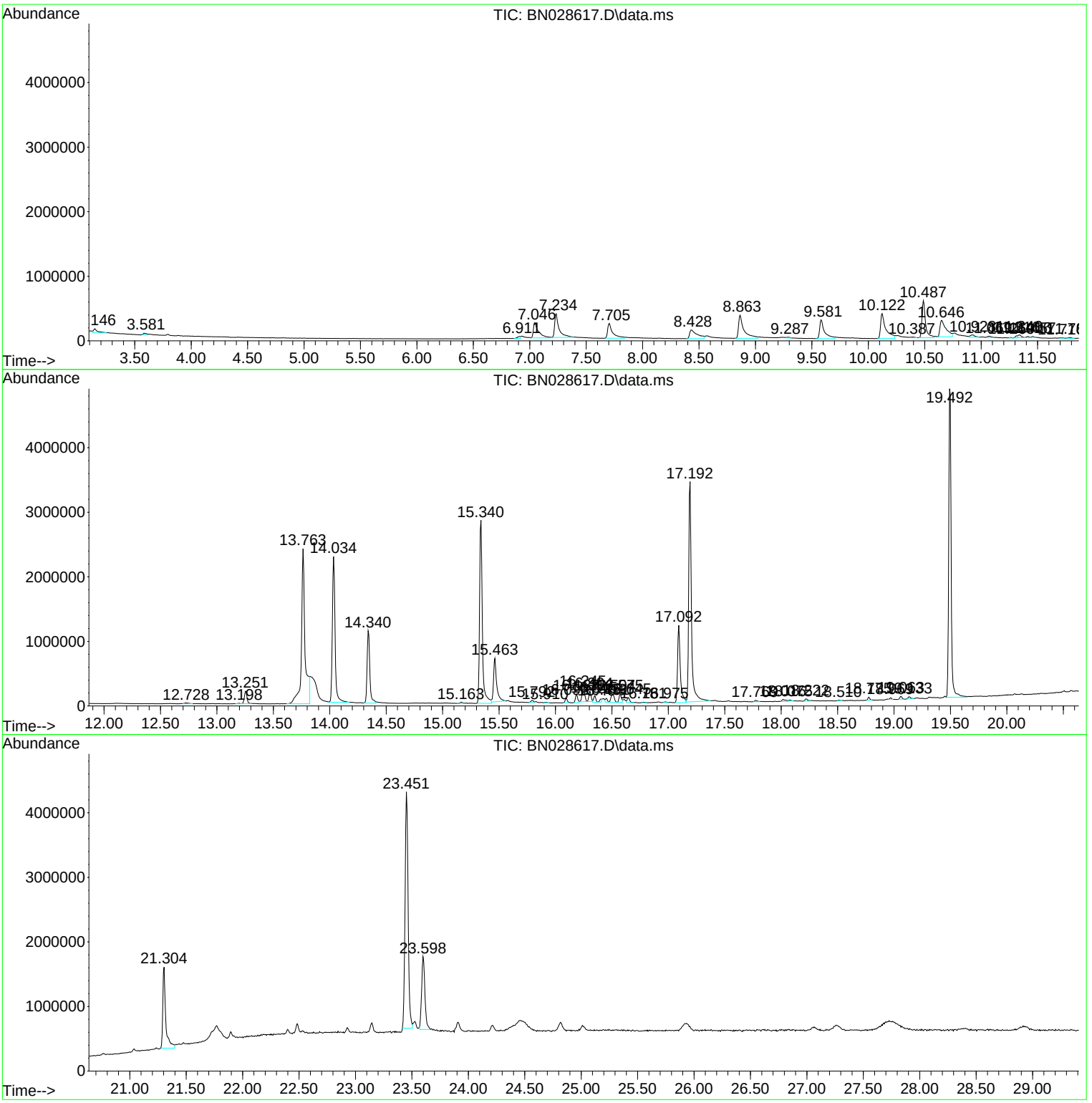
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN111423.MA.M
Quant Title : SVOA CALIBRATION

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



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Instrument :
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ClientSampleId :
GCDK4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN111423.MA.M
Quant Title : SVOA CALIBRATION

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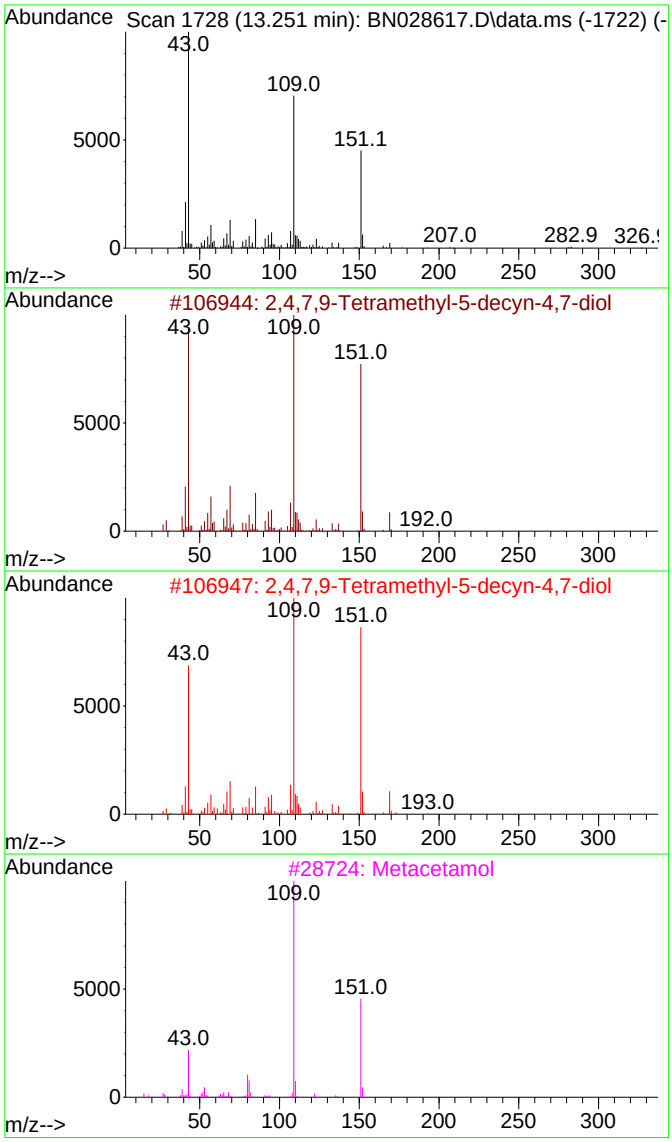
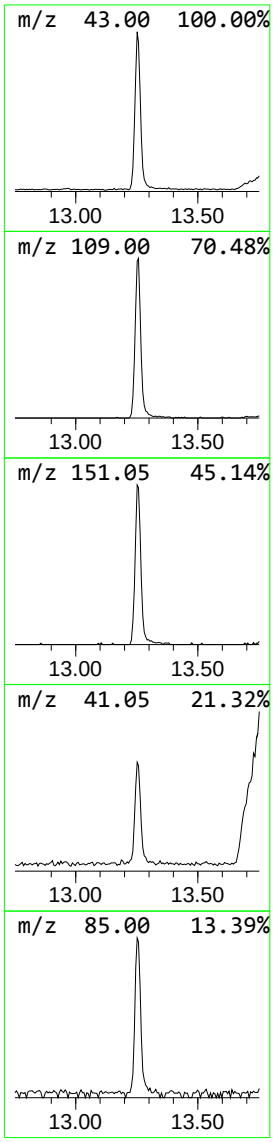
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.251	3.38 ng/ul	313187	Acenaphthene-d10	14.340

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
3	Metacetamol	151	C8H9NO2	000621-42-1	58
4	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	53
5	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	53





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ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
GCDK4

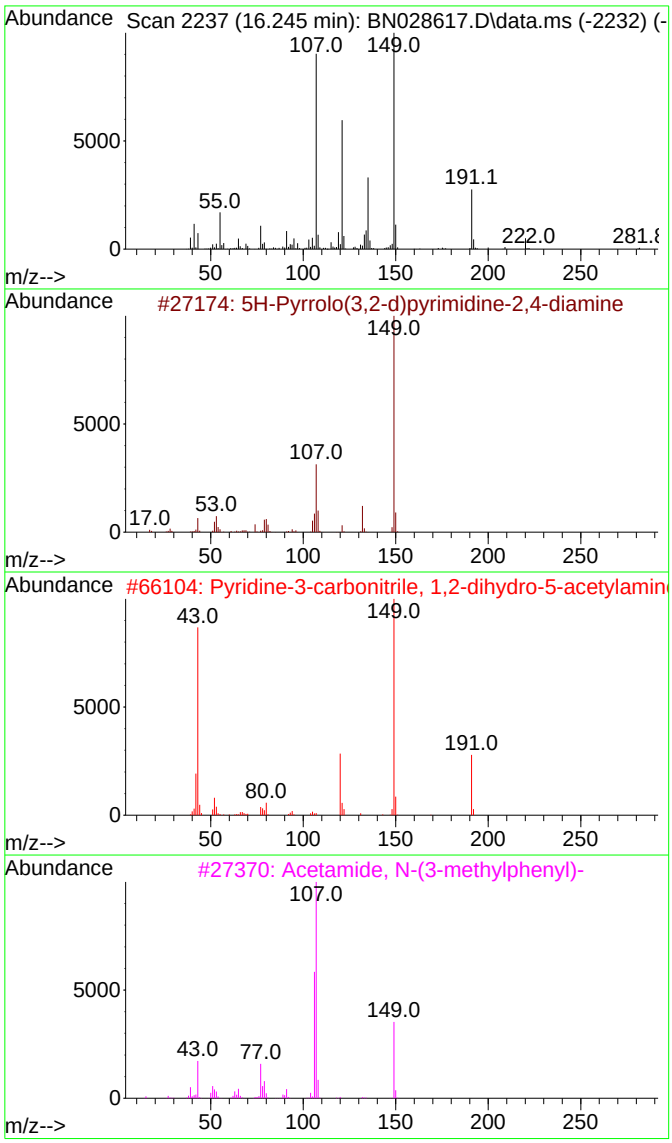
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN111423.MA.M
Quant Title : SVOA CALIBRATION

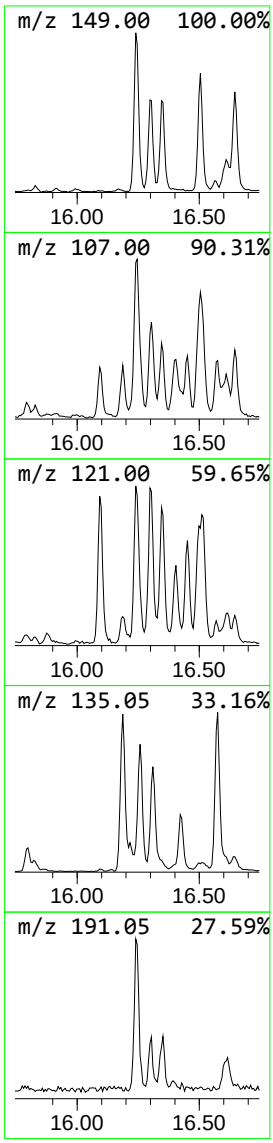
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 5H-Pyrrolo(3,2-d)pyrimidine... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.245	3.42 ng/ul	342087	Phenanthrene-d10	17.092

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-Pyrrolo(3,2-d)pyrimidine-2,4-...	149	C6H7N5	1000244-21-4	53
2	Pyridine-3-carbonitrile, 1,2-dih...	191	C9H9N3O2	220098-92-0	43
3	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	43
4	Phenol, 4-(2-methylpropyl)-	150	C10H14O	004167-74-2	38
5	Phthalic acid, propyl 2-propylph...	326	C20H22O4	1000357-01-7	35





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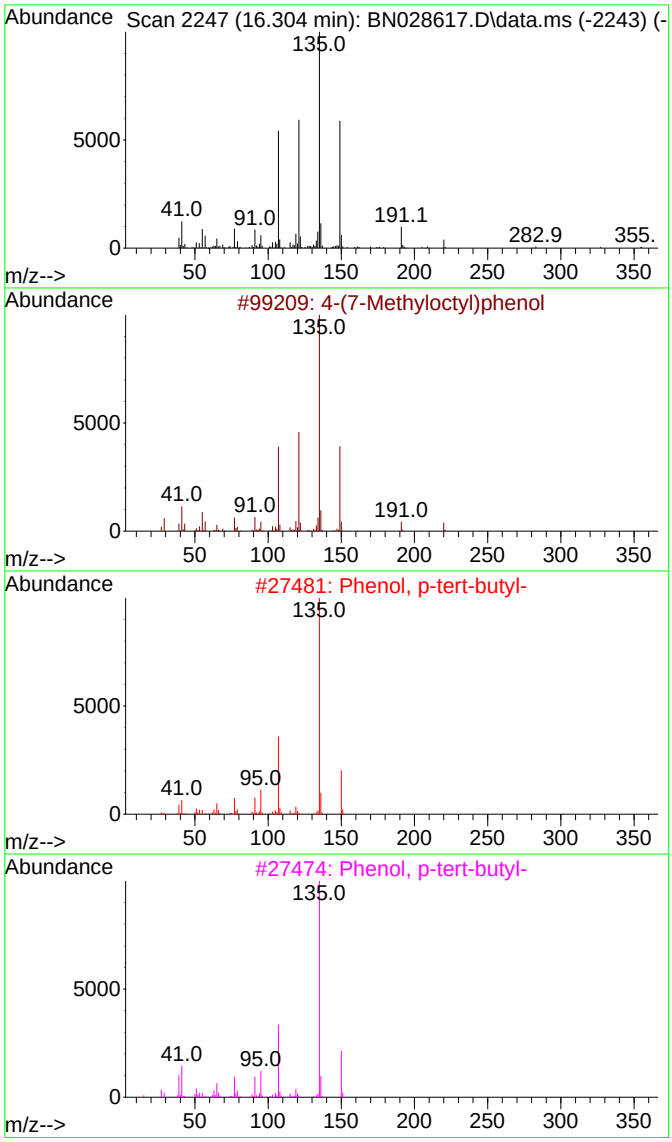
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN111423.MA.M
Quant Title : SVOA CALIBRATION

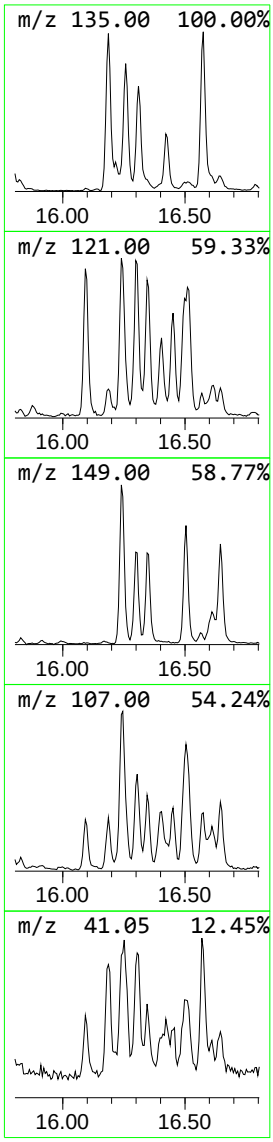
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 4-(7-Methyloctyl)phenol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.304	2.14 ng/ul	213459	Phenanthrene-d10	17.092

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(7-Methyloctyl)phenol	220	C15H24O	024518-48-7	98
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	64
3	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	64
4	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	64
5	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	52





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Sample : 05337-18
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
GCDK4

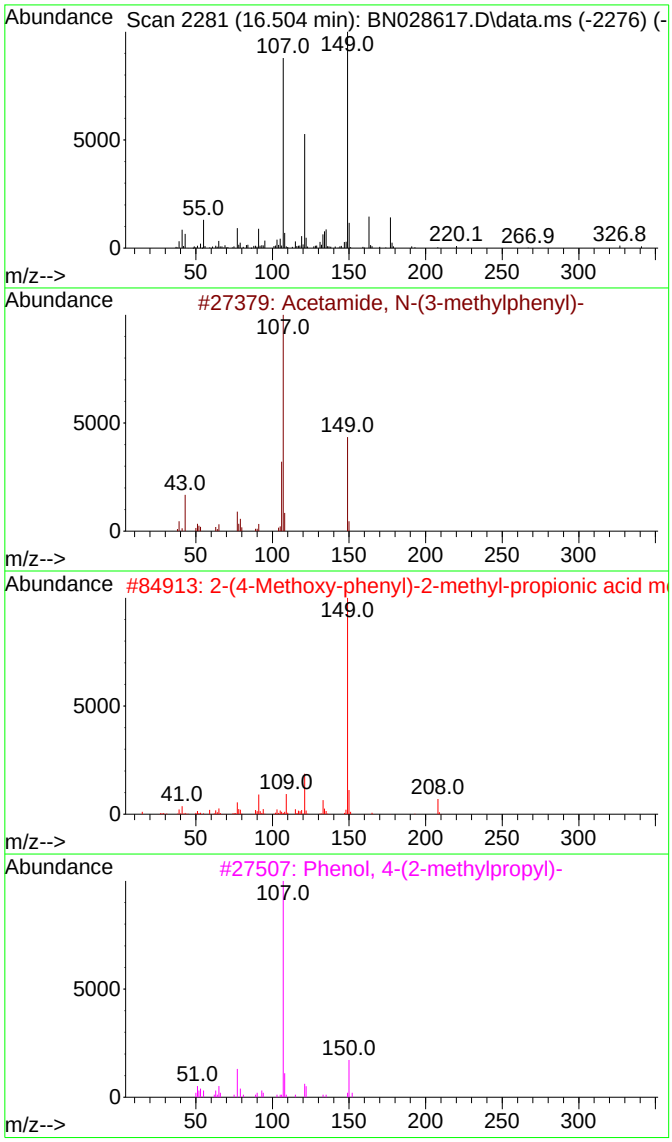
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN111423.MA.M
Quant Title : SVOA CALIBRATION

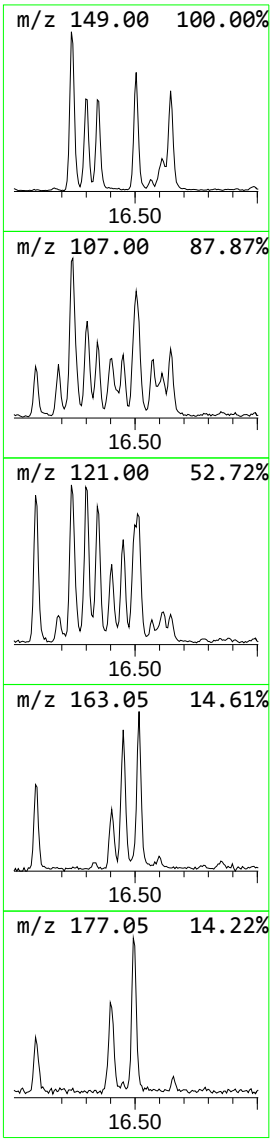
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Acetamide, N-(3-methylphenyl)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.504	2.57 ng/ul	256695	Phenanthrene-d10	17.092

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	59
2	2-(4-Methoxy-phenyl)-2-methyl-pr...	208	C12H16O3	006274-50-6	38
3	Phenol, 4-(2-methylpropyl)-	150	C10H14O	004167-74-2	38
4	5H-Pyrrolo(3,2-d)pyrimidine-2,4-...	149	C6H7N5	1000244-21-4	38
5	2H-Indol-2-one, 1,3-dihydro-5-hy...	149	C8H7NO2	003416-18-0	35





Tentatively Identified Compound (LSC) summary

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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
2,4,7,9-Tetrame...	13.251	3.4	ng/ul	313187	3	14.340	1851820	20.0
5H-Pyrrolo(3,2-...	16.245	3.4	ng/ul	342087	4	17.092	1999090	20.0
4-(7-Methylocty...	16.304	2.1	ng/ul	213459	4	17.092	1999090	20.0
Acetamide, N-(3...	16.504	2.6	ng/ul	256695	4	17.092	1999090	20.0