LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN040224\
Data File : BN030589.D
Acq On : 01 Apr 2024 15:02
Operator : MA/JU
Sample : P1925-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PMW-1(20240327)

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-BN032824.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BN030589.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.193	31	35	46	rVB	53305	84456	0.85%	0.109%
2	3.475	80	83	89	rVB4	5173	10794	0.11%	0.014%
3	3.599	102	104	124	rBV	335752	575871	5.76%	0.742%
4	3.917	154	158	164	rVB2	10158	16149	0.16%	0.021%
5	6.681	622	628	632	rBV8	5846	11280	0.11%	0.015%
6	6.864	652	659	668	rBV	275481	452548	4.53%	0.583%
7	7.034	682	688	701	rVB	891193	1406213	14.08%	1.813%
8	7.228	714	721	732	rBV	901493	1395930	13.97%	1.799%
9	7.693	792	800	818	rBV	724131	1180424	11.82%	1.521%
10	8.169	875	881	886	rVB7	6937	11709	0.12%	0.015%
11	8.393	913	919	935	rBV	777081	1276754	12.78%	1.646%
12	8.852	990	997	1006	rBV	1037123	1714760	17.17%	2.210%
13	8.952	1009	1014	1019	rVV9	5346	12412	0.12%	0.016%
14	9.016	1019	1025	1029	rVV7	8285	14043	0.14%	0.018%
15	9.263	1064	1067	1073	rVB4	7701	12153	0.12%	0.016%
16	9.569	1110	1119	1133	rBV	778349	1308111	13.10%	1.686%
17	10.010	1190	1194	1201	rVB8	5013	10024	0.10%	0.013%
18	10.099	1201	1209	1223	rBV	1290972	2141021	21.43%	2.760%
19	10.481	1263	1274	1281	rBV	1071399	1779125	17.81%	2.293%
20	10.546	1281	1285	1289	rVV5	11552	20826	0.21%	0.027%
21	10.616	1289	1297	1320	rVV	1150275	2052336	20.55%	2.645%
22	10.910	1342	1347	1352	rBV3	19550	33382	0.33%	0.043%
23	10.969	1352	1357	1364	rVB3	17829	29841	0.30%	0.038%
24	11.128	1378	1384	1390	rBV7	5315	11989	0.12%	0.015%
25	11.275	1404	1409	1413	rBV3	13221	18651	0.19%	0.024%
26	11.410	1422	1432	1449	rBV	726484	1405061	14.07%	1.811%
27	11.828	1494	1503	1508	rBV	63231	112768	1.13%	0.145%
28	12.069	1539	1544	1551	rVB	23734	40513	0.41%	0.052%
29	12.269	1572	1578	1585	rBV3	14697	29066	0.29%	0.037%
30	13.157	1724	1729	1732	rBV4	10317	18226	0.18%	0.023%
31	13.240	1737	1743	1748	rVV2	19790	34116	0.34%	0.044%
32	13.310	1750	1755	1760	rVB7	7132	14087	0.14%	0.018%
33	13.381	1763	1767	1771	rVV6	6913	10136	0.10%	0.013%
34	13.440	1771	1777	1783	rVV4	6387	15148	0.15%	0.020%
35	13.504	1785	1788	1797	rVB6	7737	14097	0.14%	0.018%
36	13.657	1804	1814	1821	rBV	62077	105293	1.05%	0.136%

LSC Area Percent Report

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Operator : MA/JU
Sample : P1925-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PMW-1(20240327)

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-BN032824.MA.M
Title : SVOA CALIBRATION

37	13.757	1824	1831	1839	rVV	2486968	3558492	35.62%	4.587%
38	13.828	1839	1843	1849	rVB	143476	190502	1.91%	0.246%
39	14.028	1867	1877	1886	rBV	2888774	4361744	43.66%	5.622%
40	14.128	1890	1894	1899	rVB3	11736	19960	0.20%	0.026%
41	14.340	1919	1930	1937	rBV2	1718748	2608352	26.11%	3.362%
42	14.416	1941	1943	1950	rVB7	8956	15443	0.15%	0.020%
43	14.534	1957	1963	1981	rBV2	281922	471075	4.72%	0.607%
44	14.757	1998	2001	2006	rVB5	12920	19016	0.19%	0.025%
45	14.834	2006	2014	2020	rBV	94413	155066	1.55%	0.200%
46	15.093	2053	2058	2063	rBV	17007	23978	0.24%	0.031%
47	15.240	2077	2083	2087	rBV8	5413	10357	0.10%	0.013%
48	15.334	2092	2099	2112	rBV	3834886	5397913	54.04%	6.958%
49	15.445	2112	2118	2125	rBV	946847	1323983	13.25%	1.707%
50	15.557	2131	2137	2150	rBV2	171027	288543	2.89%	0.372%
51	15.904	2191	2196	2200	rBV7	9591	15289	0.15%	0.020%
52	15.987	2200	2210	2214	rBV	5210337	9989315	100.00%	12.876%
53	16.122	2229	2233	2244	rVB	204383	319478	3.20%	0.412%
54	16.498	2295	2297	2301	rVB4	10212	10891	0.11%	0.014%
55	16.669	2321	2326	2333	rVB	53789	77503	0.78%	0.100%
56	16.810	2346	2350	2355	rVB9	6420	9991	0.10%	0.013%
57	17.010	2379	2384	2390	rBV	86672	145238	1.45%	0.187%
58	17.087	2390	2397	2407	rVB	2036449	2976882	29.80%	3.837%
59	17.187	2407	2414	2425	rBV2	4069792	6014709	60.21%	7.753%
60	17.922	2536	2539	2543	rVB5	7998	11491	0.12%	0.015%
61	17.986	2545	2550	2559	rBV2	121315	190497	1.91%	0.246%
62	18.069	2559	2564	2569	rVB	72950	105830	1.06%	0.136%
63	18.428	2622	2625	2628	rVB5	10303	12473	0.12%	0.016%
64	18.739	2676	2678	2683	rVB5	11609	13457	0.13%	0.017%
65	18.928	2706	2710	2715	rBV	27612	43490	0.44%	0.056%
66	18.975	2715	2718	2722	rVV4	19929	26868	0.27%	0.035%
67	19.045	2726	2730	2734	rVV2	69792	92542	0.93%	0.119%
68	19.116	2738	2742	2746	rVV	74107	105973	1.06%	0.137%
69	19.151	2746	2748	2752	rVB5	14505	18656	0.19%	0.024%
70	19.275	2765	2769	2774	rBV	75832	102657	1.03%	0.132%
71	19.486	2798	2805	2812	rBV	5245137	7184168	71.92%	9.260%
72	21.016	3062	3065	3071	rBV5	39566	59046	0.59%	0.076%
73	21.322	3111	3117	3127	rBV	2279623	3402459	34.06%	4.386%
74	24.069	3574	3584	3598	rBV2	3027841	7316435	73.24%	9.430%
75	24.263	3609	3617	3636	rVB	1360851	3513911	35.18%	4.529%

LSC Area Percent Report

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Data File : BN030589.D
Acq On : 01 Apr 2024 15:02
Operator : MA/JU
Sample : P1925-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PMW-1(20240327)

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

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Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN032824.MA.M
Title : SVOA CALIBRATION

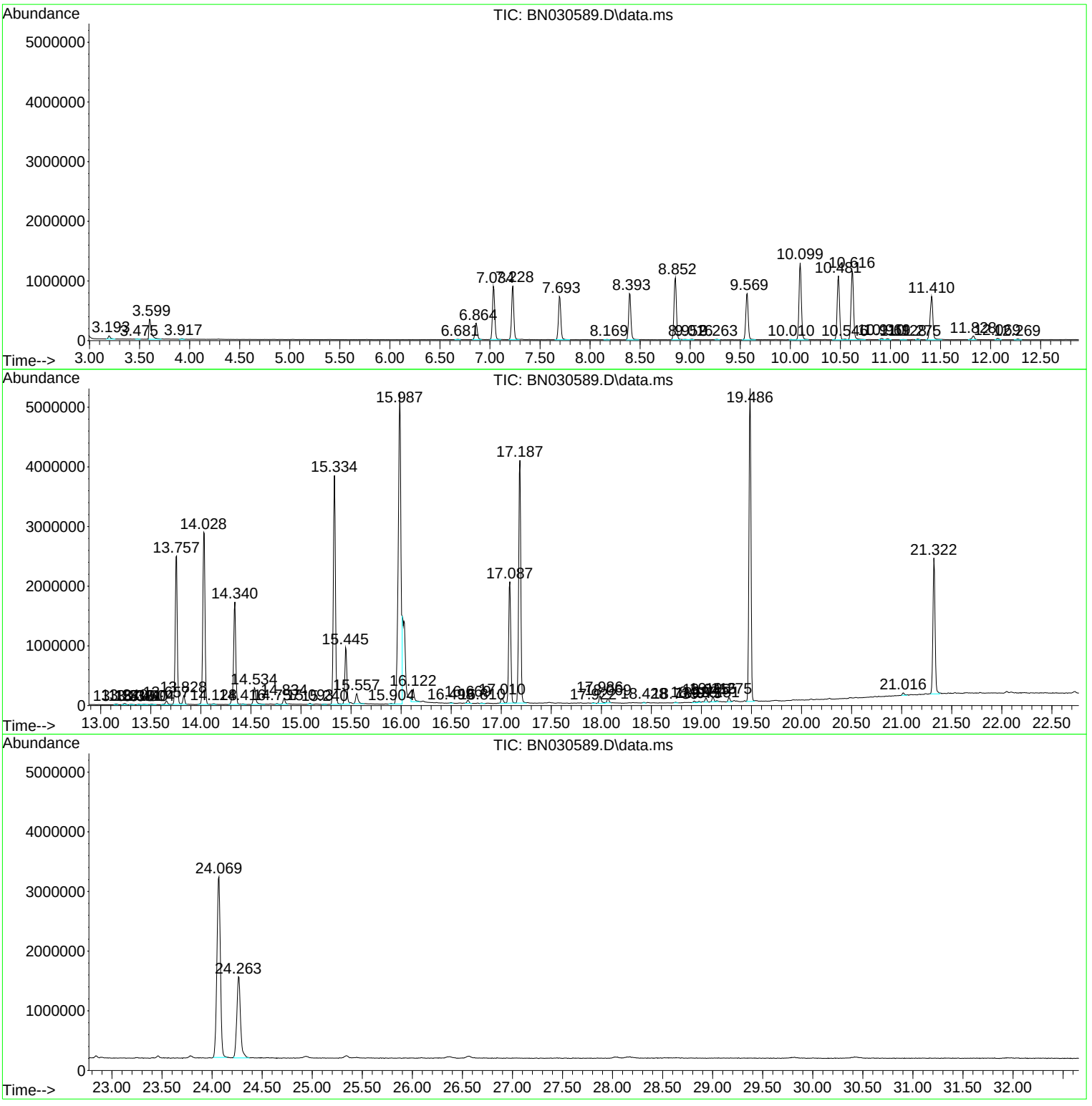
Sum of corrected areas: 77582986

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN040224\
Data File : BN030589.D
Acq On : 01 Apr 2024 15:02
Operator : MA/JU
Sample : P1925-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PMW-1(20240327)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN032824.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\BN040224\
Data File : BN030589.D
Acq On : 01 Apr 2024 15:02
Operator : MA/JU
Sample : P1925-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PMW-1(20240327)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN032824.MA.M
Quant Title : SVOA CALIBRATION

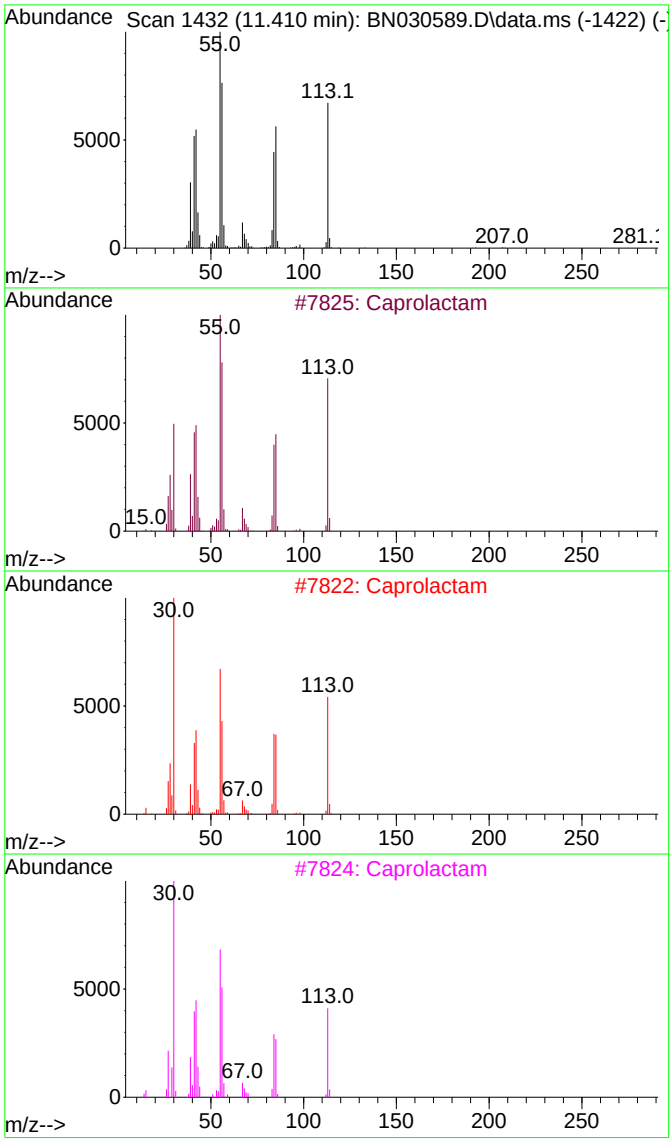
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

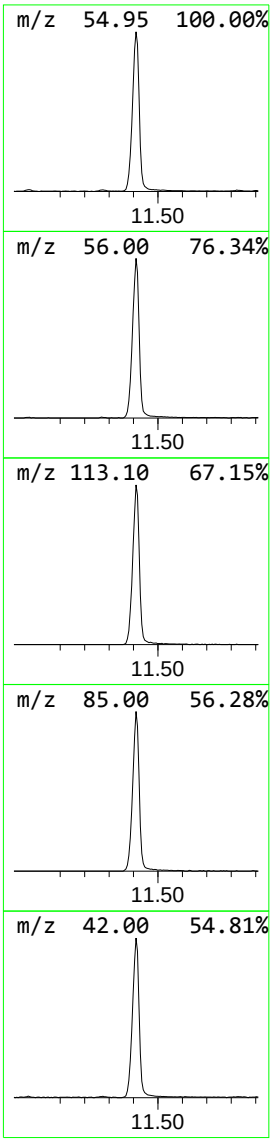
****

Peak Number 1 Capro lactam Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.410	15.80 ng/ul	1405060	Naphthalene-d8	10.481

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caprolactam	113	C6H11NO	000105-60-2	94
2	Caprolactam	113	C6H11NO	000105-60-2	94
3	Caprolactam	113	C6H11NO	000105-60-2	90
4	Caprolactam	113	C6H11NO	000105-60-2	74
5	1-Hexene	84	C6H12	000592-41-6	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN040224\
Data File : BN030589.D
Acq On : 01 Apr 2024 15:02
Operator : MA/JU
Sample : P1925-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PMW-1(20240327)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN032824.MA.M
Quant Title : SVOA CALIBRATION

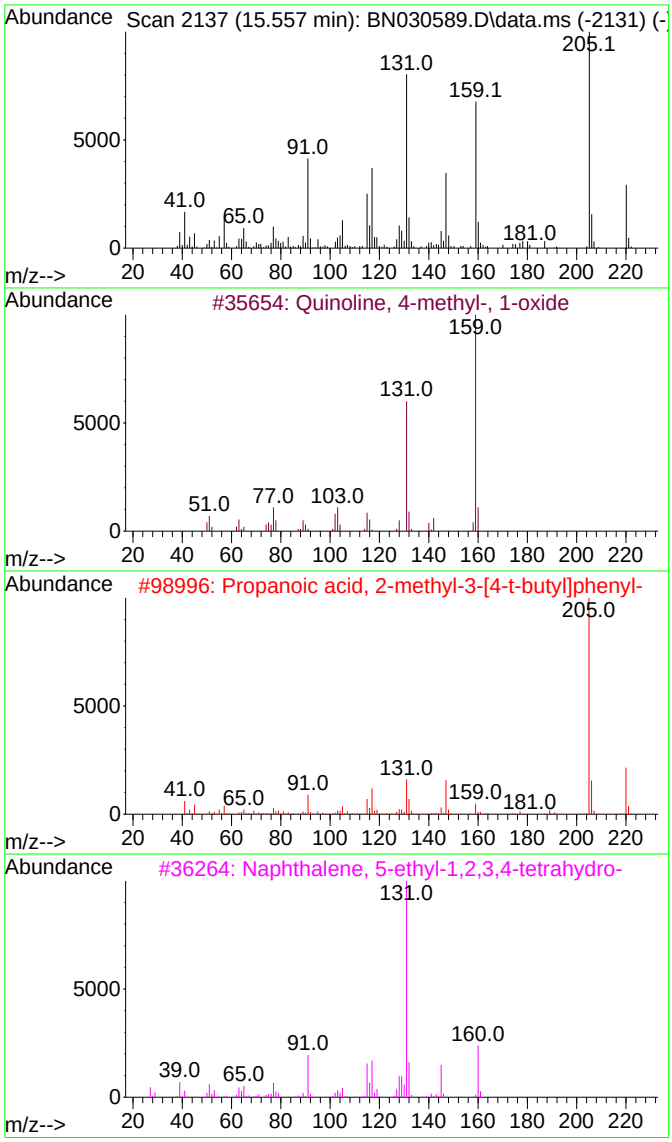
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

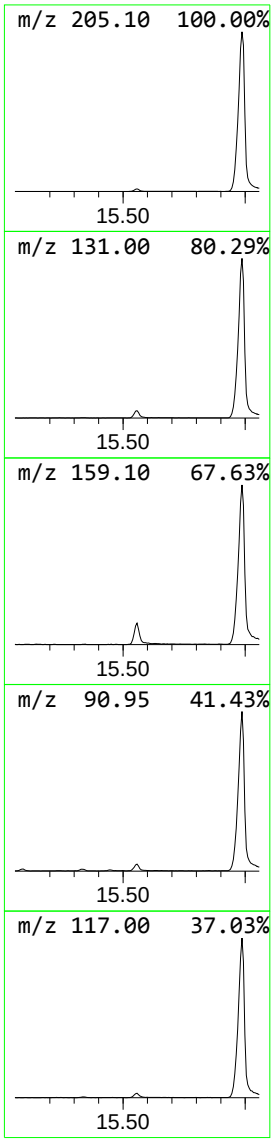
****

Peak Number 2 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.557	2.21 ng/ul	288543	Acenaphthene-d10	14.340

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Quinoline, 4-methyl-, 1-oxide	159	C10H9NO	004053-40-1	45
2	Propanoic acid, 2-methyl-3-[4-t-...	220	C14H20O2	1000131-87-0	43
3	Naphthalene, 5-ethyl-1,2,3,4-tet...	160	C12H16	042775-75-7	42
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	160	C12H16	078920-29-3	42
5	4(1H)-Quinolinone, 1-methyl-	159	C10H9NO	000083-54-5	41





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN040224\
Data File : BN030589.D
Acq On : 01 Apr 2024 15:02
Operator : MA/JU
Sample : P1925-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PMW-1(20240327)

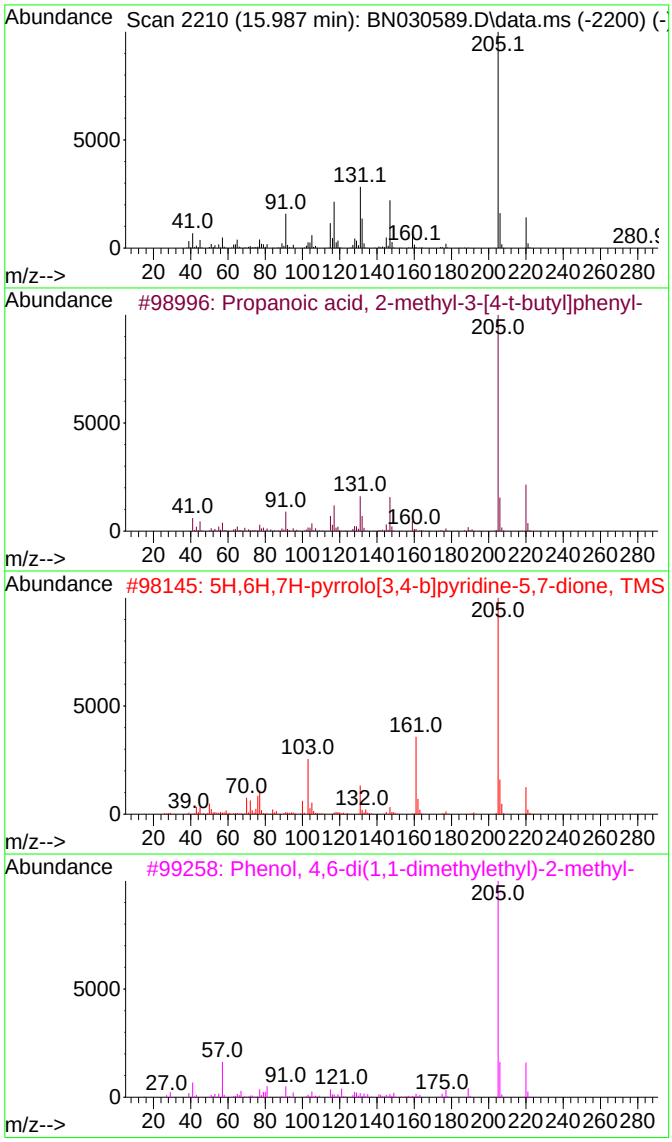
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN032824.MA.M
Quant Title : SVOA CALIBRATION

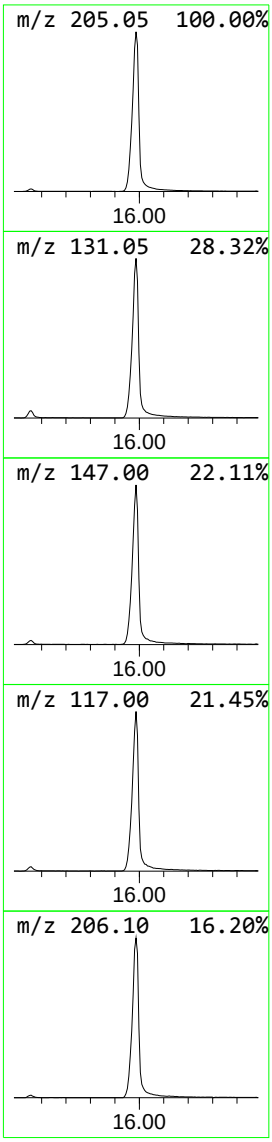
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Propanoic acid, 2-methyl-3-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.987	67.11 ng/ul	9989320	Phenanthrene-d10	17.087

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-3-[4-t-...	220	C14H20O2	1000131-87-0	94
2	5H,6H,7H-pyrrolo[3,4-b]pyridine-...	220	C10H12N2O2Si	1000485-20-1	47
3	Phenol, 4,6-di(1,1-dimethylethyl...	220	C15H24O	000616-55-7	43
4	5-(1H-Pyrrol-3-ylmethylene)-pyri...	205	C9H7N3O3	1000318-16-3	38
5	Trimethyl-3,4-methylenedioxychro...	220	C13H16O3	1000378-97-7	38





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN032824.MA.M
Quant Title : SVOA CALIBRATION

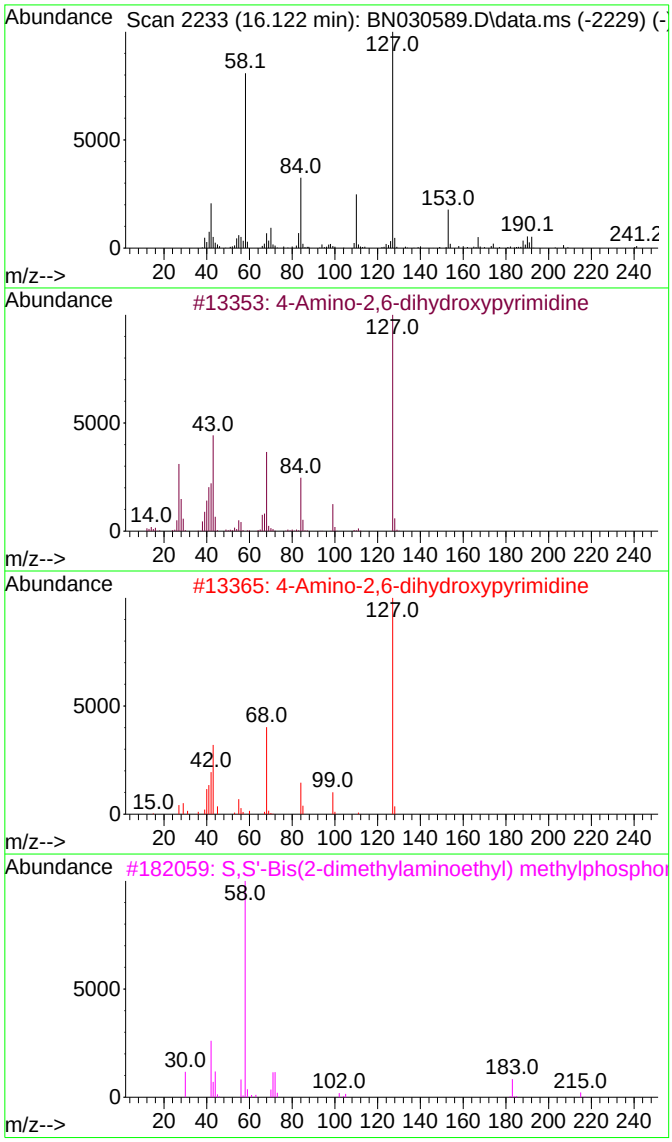
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

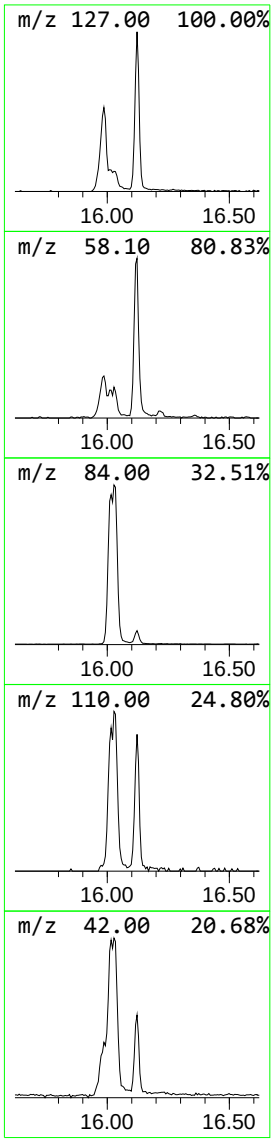
****

Peak Number 4 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.122	2.15 ng/ul	319478	Phenanthrene-d10	17.087

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Amino-2,6-dihydroxypyrimidine	127	C4H5N3O2	000873-83-6	35
2	4-Amino-2,6-dihydroxypyrimidine	127	C4H5N3O2	000873-83-6	27
3	S,S'-Bis(2-dimethylaminoethyl) m...	286	C9H23N2PS3	170425-22-6	27
4	1-Heptanamine, N,N-dimethyl-	143	C9H21N	005277-11-2	27
5	1-Methylheptyl isopropylphosphon...	238	C11H24FO2P	1000273-54-8	25





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN032824.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
Capro lactam	11.410	15.8	ng/ul	1405060	2	10.481	1779130	20.0
unknown-01	15.557	2.2	ng/ul	288543	3	14.340	2608350	20.0
Propanoic acid,...	15.987	67.1	ng/ul	9989320	4	17.087	2976880	20.0
unknown-02	16.122	2.1	ng/ul	319478	4	17.087	2976880	20.0