LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037739.D
Acq On : 26 Nov 2022 18:43
Operator : CG/JU
Sample : N5602-16
Misc :
ALS Vial : 51 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AG8

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_M\Methods\SFAM-EPA-BM112322.M
Title : SVOA CALIBRATION

Signal : TIC: BM037739.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.434	4	8	13	rBV	58166	77010	0.81%	0.080%
2	3.481	13	16	19	rVB3	17687	20341	0.21%	0.021%
3	3.781	64	67	75	rVB7	14458	33808	0.35%	0.035%
4	3.875	79	83	97	rBV	381389	655865	6.87%	0.678%
5	4.040	107	111	115	rBV6	9022	15295	0.16%	0.016%
6	4.110	119	123	128	rVB	36633	56326	0.59%	0.058%
7	4.210	135	140	145	rBV	88144	133149	1.39%	0.138%
8	4.252	145	147	151	rVB2	18529	19067	0.20%	0.020%
9	4.334	158	161	167	rVB6	9662	15477	0.16%	0.016%
10	4.675	215	219	225	rVB2	21157	38799	0.41%	0.040%
11	5.169	299	303	310	rBV	197604	269800	2.83%	0.279%
12	5.510	354	361	366	rBV6	11094	18960	0.20%	0.020%
13	5.763	398	404	409	rBV6	11173	19507	0.20%	0.020%
14	6.134	461	467	470	rBV5	12156	23766	0.25%	0.025%
15	6.369	501	507	511	rBV8	8490	14696	0.15%	0.015%
16	6.793	569	579	582	rVV10	6214	19485	0.20%	0.020%
17	6.863	585	591	594	rBV4	9478	13795	0.14%	0.014%
18	7.257	648	658	664	rBV	478107	727377	7.62%	0.752%
19	7.351	670	674	681	rBV2	8196	16938	0.18%	0.018%
20	7.428	681	687	703	rBV	1297478	2064637	21.62%	2.135%
21	7.634	715	722	733	rBV	1313060	2077130	21.75%	2.148%
22	7.957	772	777	784	rVB4	16627	27534	0.29%	0.028%
23	8.110	796	803	810	rBV	920683	1421191	14.88%	1.470%
24	8.204	810	819	826	rVV6	34252	67172	0.70%	0.069%
25	8.463	858	863	867	rBV6	12797	18628	0.20%	0.019%
26	8.557	874	879	885	rVB7	19367	41500	0.43%	0.043%
27	8.657	887	896	898	rBV	25684	45920	0.48%	0.047%
28	8.757	908	913	917	rBV3	24061	42047	0.44%	0.043%
29	8.816	917	923	930	rVV	1256332	1952761	20.45%	2.020%
30	8.910	930	939	943	rVV6	18956	42168	0.44%	0.044%
31	8.945	943	945	950	rVV4	15919	27141	0.28%	0.028%
32	9.004	951	955	961	rVB8	17736	31814	0.33%	0.033%
33	9.110	969	973	979	rVB	46709	70317	0.74%	0.073%
34	9.222	988	992	995	rVB2	19717	24370	0.26%	0.025%
35	9.281	995	1002	1009	rBV	1760906	2797586	29.29%	2.893%
36	9.351	1009	1014	1023	rVB5	31429	77079	0.81%	0.080%

LSC Area Percent Report

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Operator : CG/JU
Sample : N5602-16
Misc :
ALS Vial : 51 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AG8

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_M\Methods\SFAM-EPA-BM112322.M
Title : SVOA CALIBRATION

37	9.439	1023	1029	1033	rBV9	10841	27404	0.29%	0.028%
38	9.504	1034	1040	1044	rVV3	27823	49925	0.52%	0.052%
39	9.722	1068	1077	1085	rBV	102121	203333	2.13%	0.210%
40	9.786	1085	1088	1092	rVV5	12574	19591	0.21%	0.020%
41	9.904	1102	1108	1110	rBV6	11196	19690	0.21%	0.020%
42	10.004	1118	1125	1132	rBV	1370448	2233560	23.39%	2.310%
43	10.057	1132	1134	1140	rVB6	12211	18834	0.20%	0.019%
44	10.216	1155	1161	1169	rVB6	20342	48180	0.50%	0.050%
45	10.328	1176	1180	1188	rBV9	26388	52087	0.55%	0.054%
46	10.410	1189	1194	1197	rBV5	15757	23450	0.25%	0.024%
47	10.481	1202	1206	1209	rVV5	32445	57594	0.60%	0.060%
48	10.545	1210	1217	1225	rVB	1976222	3228824	33.81%	3.339%
49	10.686	1236	1241	1242	rBV5	21055	31684	0.33%	0.033%
50	10.751	1249	1252	1260	rVB10	15790	34133	0.36%	0.035%
51	10.822	1260	1264	1268	rBV7	8216	15277	0.16%	0.016%
52	10.869	1270	1272	1276	rVB4	13176	14668	0.15%	0.015%
53	10.933	1276	1283	1289	rBV	1370344	2258798	23.65%	2.336%
54	10.986	1289	1292	1298	rVB6	17222	27110	0.28%	0.028%
55	11.069	1298	1306	1315	rBV	1123773	2046019	21.42%	2.116%
56	11.210	1327	1330	1339	rVB2	43104	87740	0.92%	0.091%
57	11.351	1349	1354	1358	rBV3	39371	57642	0.60%	0.060%
58	11.498	1372	1379	1381	rBV3	64778	115413	1.21%	0.119%
59	11.586	1389	1394	1397	rBV7	18762	30726	0.32%	0.032%
60	11.628	1397	1401	1407	rVB5	27279	46208	0.48%	0.048%
61	11.710	1411	1415	1419	rBV5	22433	38105	0.40%	0.039%
62	11.751	1419	1422	1426	rBV5	16597	21359	0.22%	0.022%
63	11.810	1426	1432	1438	rBV3	56947	123661	1.29%	0.128%
64	12.257	1498	1508	1513	rBV	228820	397097	4.16%	0.411%
65	12.316	1514	1518	1526	rVB6	41305	89138	0.93%	0.092%
66	12.445	1536	1540	1543	rBV5	27053	38699	0.41%	0.040%
67	12.504	1547	1550	1555	rVB3	27241	42885	0.45%	0.044%
68	12.639	1570	1573	1577	rVB3	33631	42111	0.44%	0.044%
69	12.769	1591	1595	1597	rBV4	34206	52404	0.55%	0.054%
70	12.798	1598	1600	1608	rVB7	44439	70503	0.74%	0.073%
71	12.880	1610	1614	1618	rBV4	65438	105115	1.10%	0.109%
72	13.022	1634	1638	1644	rBV7	43882	113637	1.19%	0.118%
73	13.116	1651	1654	1662	rVB10	37791	88107	0.92%	0.091%
74	13.327	1687	1690	1695	rVB5	60622	91696	0.96%	0.095%
75	13.733	1756	1759	1763	rBV3	43380	59223	0.62%	0.061%
76	13.922	1787	1791	1794	rBV	103081	151751	1.59%	0.157%

LSC Area Percent Report

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Acq On : 26 Nov 2022 18:43
Operator : CG/JU
Sample : N5602-16
Misc :
ALS Vial : 51 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AG8

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_M\Methods\SFAM-EPA-BM112322.M
Title : SVOA CALIBRATION

77	14.004	1798	1805	1816	rVV	1456188	2590224	27.12%	2.679%
78	14.145	1823	1829	1834	rVB	3890259	5355284	56.08%	5.539%
79	14.433	1872	1878	1888	rVB	4446885	6350559	66.50%	6.568%
80	14.539	1892	1896	1906	rVB	321130	485538	5.08%	0.502%
81	14.651	1911	1915	1922	rVB3	117652	209224	2.19%	0.216%
82	14.733	1923	1929	1935	rBV	2206316	3281446	34.36%	3.394%
83	14.874	1949	1953	1957	rBV4	137278	255691	2.68%	0.264%
84	14.921	1957	1961	1972	rVB	588577	901315	9.44%	0.932%
85	15.080	1985	1988	1995	rBV8	62335	115163	1.21%	0.119%
86	15.204	2006	2009	2010	rBV2	61632	76253	0.80%	0.079%
87	15.721	2091	2097	2103	rBV	5675912	7918093	82.91%	8.189%
88	15.827	2110	2115	2120	rBV	2052292	2914299	30.52%	3.014%
89	16.227	2180	2183	2189	rBV4	143984	222902	2.33%	0.231%
90	17.474	2390	2395	2400	rVB	2843921	3922663	41.08%	4.057%
91	17.574	2406	2412	2418	rVB	6008381	8526456	89.28%	8.819%
92	17.833	2453	2456	2466	rVB2	220777	349770	3.66%	0.362%
93	17.957	2474	2477	2481	rVB	222613	287696	3.01%	0.298%
94	18.357	2541	2545	2553	rBV	377088	587956	6.16%	0.608%
95	19.621	2757	2760	2766	rVB	447353	560694	5.87%	0.580%
96	19.851	2794	2799	2804	rBV	7242869	9549794	100.00%	9.877%
97	19.968	2814	2819	2824	rBV	2179288	2693909	28.21%	2.786%
98	21.639	3098	3103	3110	rBV	2842294	3749852	39.27%	3.878%
99	23.968	3492	3499	3508	rVB2	3626765	7482122	78.35%	7.738%
100	24.127	3520	3526	3534	rVB2	1469614	3008421	31.50%	3.111%

Sum of corrected areas: 96687161

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037739.D
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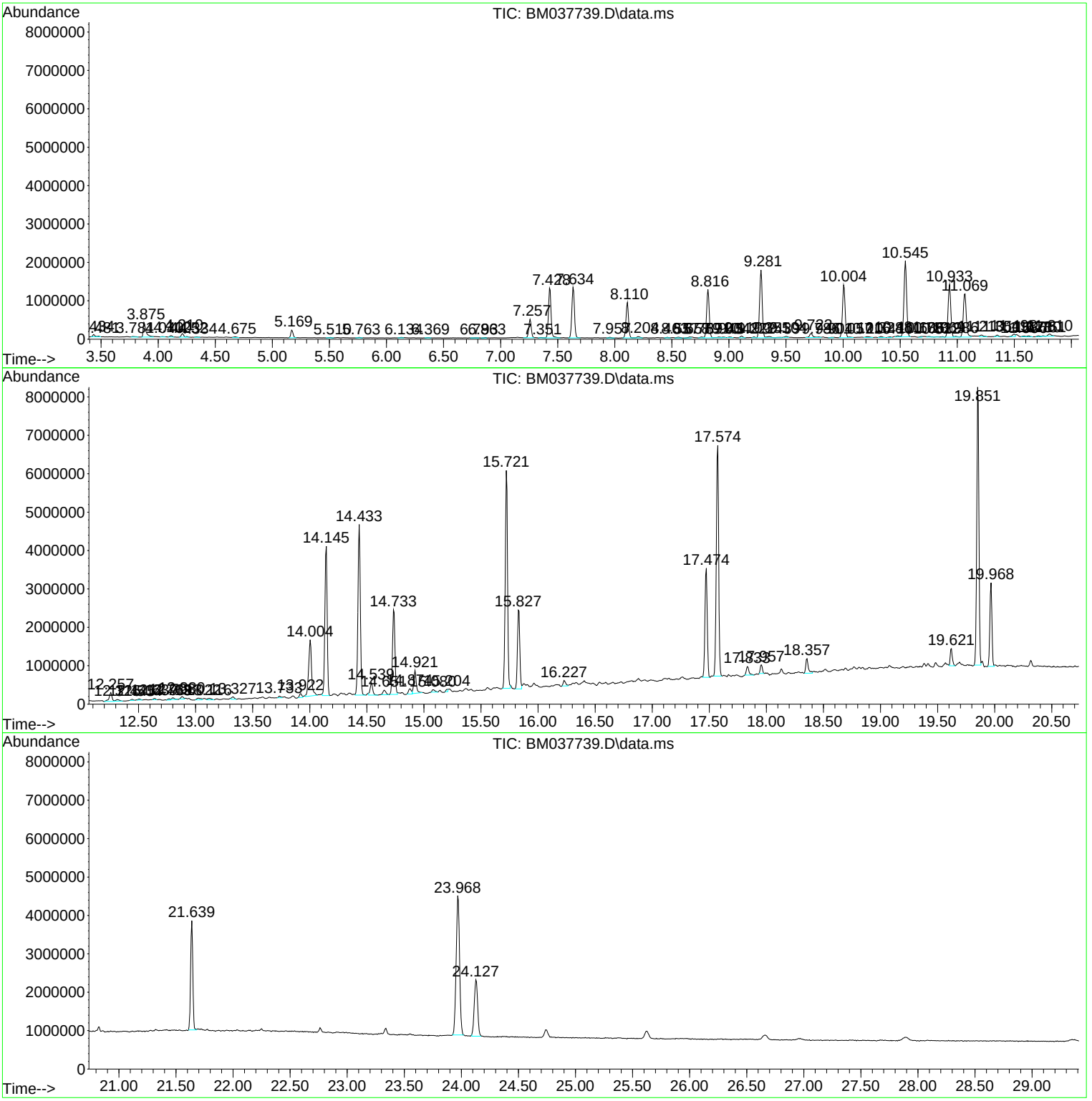
ALS Vial : 51 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AG8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037739.D
Acq On : 26 Nov 2022 18:43
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Sample : N5602-16
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Instrument :
BNA_M
ClientSampleId :
C0AG8

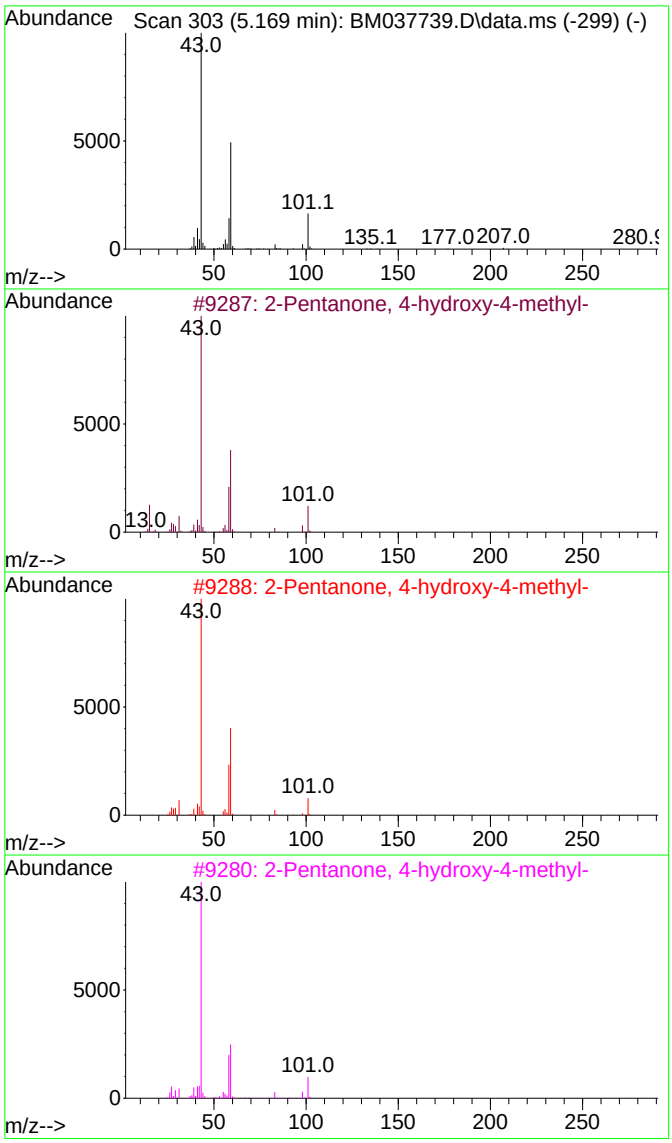
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

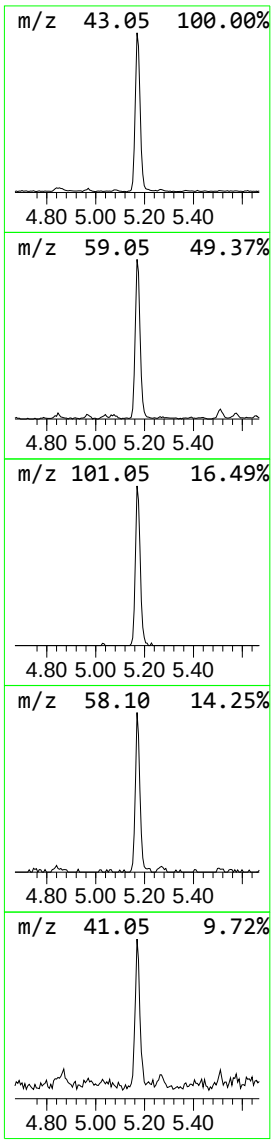
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.169	3.80 ng/ul	269800	1,4-Dichlorobenzene-d4	8.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
4	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037739.D
Acq On : 26 Nov 2022 18:43
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ALS Vial : 51 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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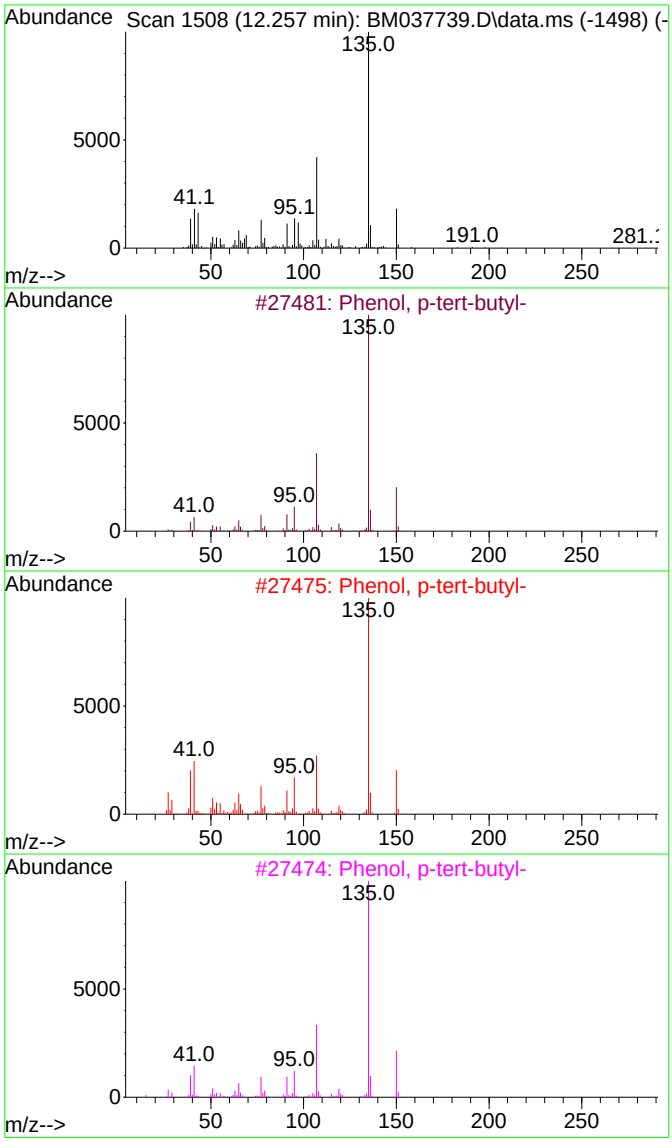
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

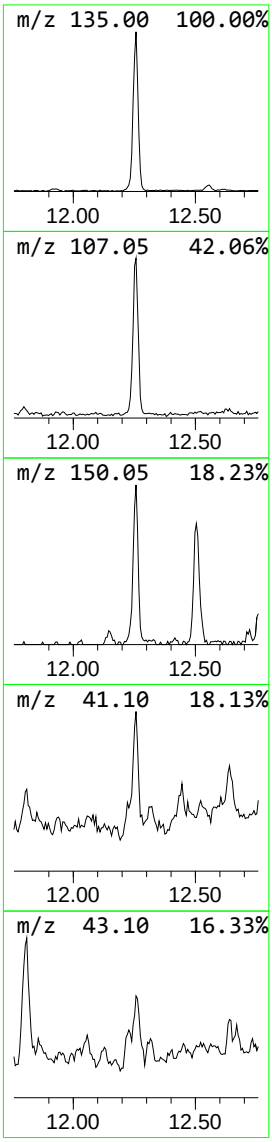
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Phenol, p-tert-butyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.257	3.52 ng/ul	397097	Naphthalene-d8	10.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	94
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	94
3	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	94
4	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	87
5	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
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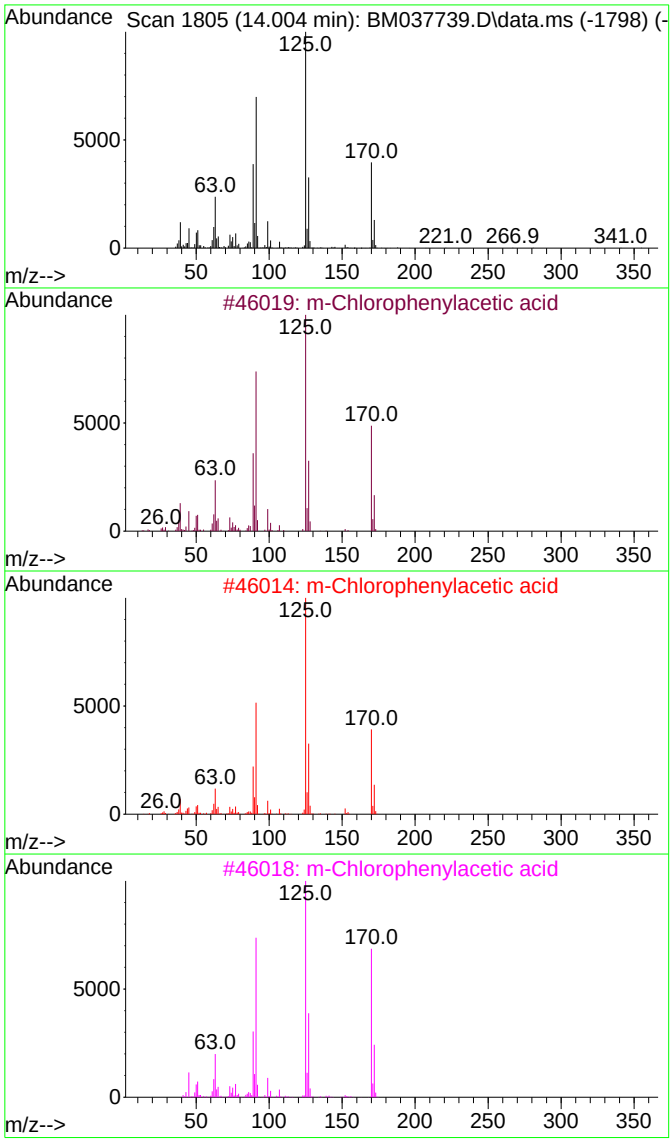
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

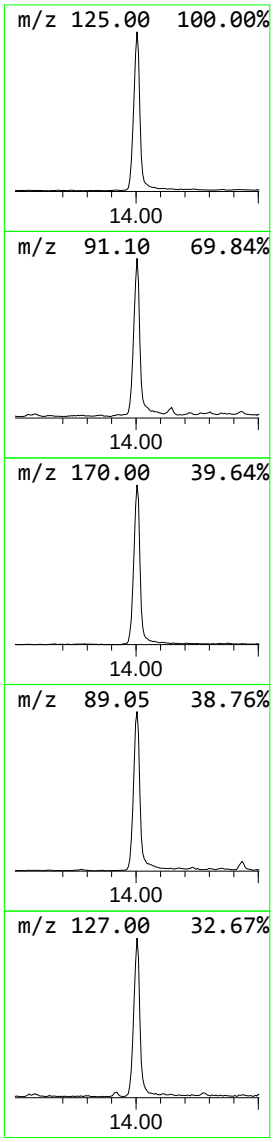
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 m-Chlorophenylacetic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.004	15.79 ng/ul	2590220	Acenaphthene-d10	14.733

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	m-Chlorophenylacetic acid	170	C8H7ClO2	001878-65-5	97
2	m-Chlorophenylacetic acid	170	C8H7ClO2	001878-65-5	96
3	m-Chlorophenylacetic acid	170	C8H7ClO2	001878-65-5	96
4	Benzeneacetic acid, 4-chloro-	170	C8H7ClO2	001878-66-6	94
5	Benzeneacetic acid, 4-chloro-	170	C8H7ClO2	001878-66-6	94





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

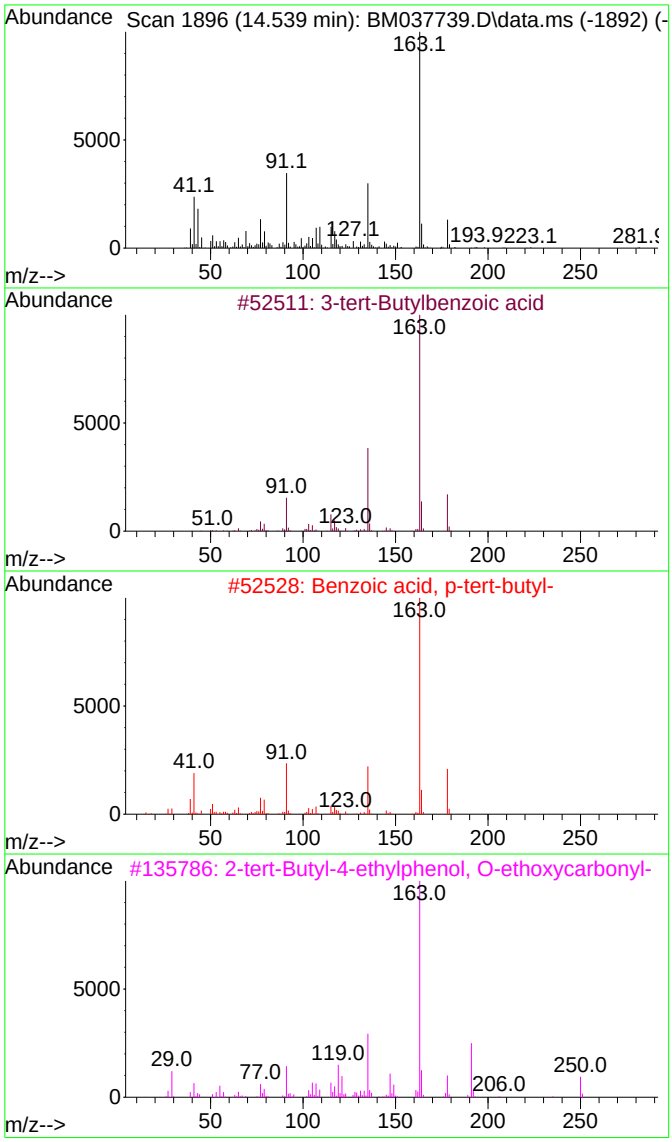
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

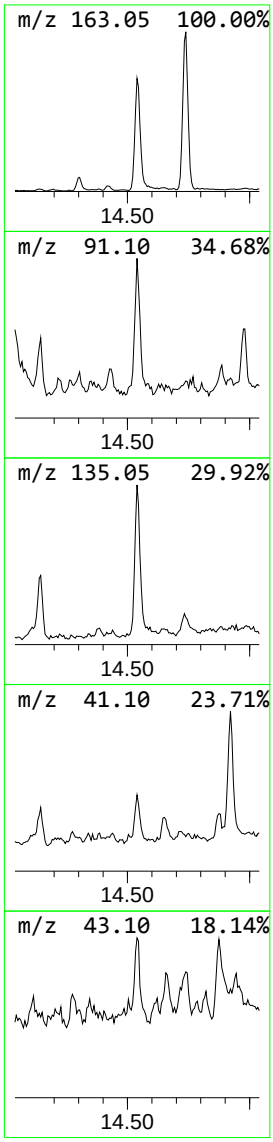
****

Peak Number 4 3-tert-Butylbenzoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.539	2.96 ng/ul	485538	Acenaphthene-d10	14.733

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-tert-Butylbenzoic acid	178	C11H14O2	007498-54-6	94
2	Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	93
3	2-tert-Butyl-4-ethylphenol, O-et...	250	C15H22O3	1000487-42-3	72
4	Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	62
5	6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037739.D
Acq On : 26 Nov 2022 18:43
Operator : CG/JU
Sample : N5602-16
Misc :
ALS Vial : 51 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AG8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

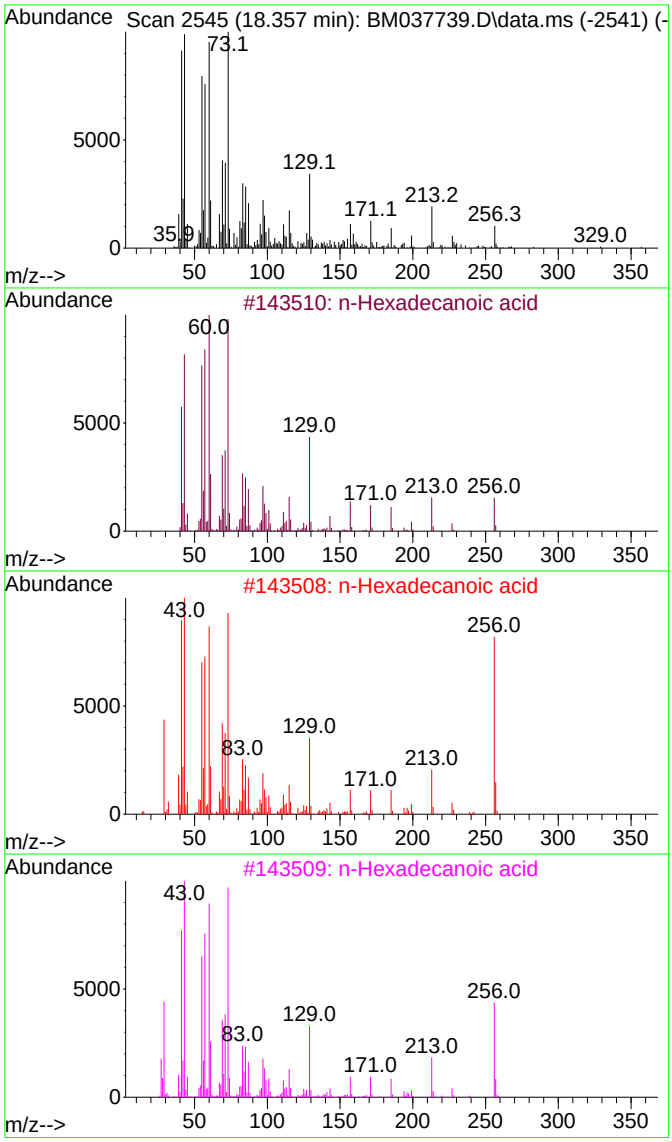
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

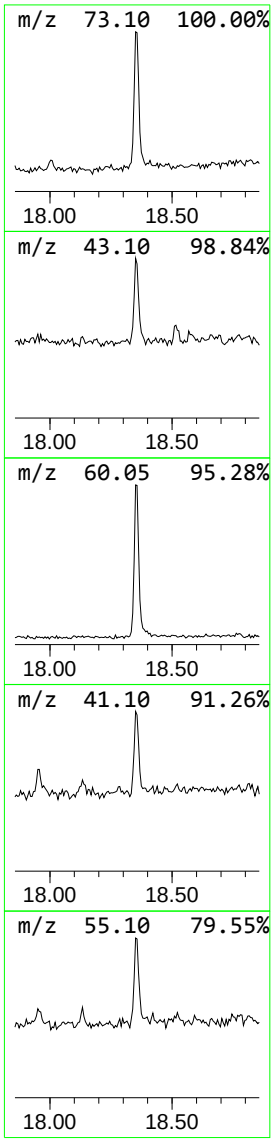
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.357	3.00 ng/ul	587956	Phenanthrene-d10	17.474

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	90





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Data File : BM037739.D
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Operator : CG/JU
Sample : N5602-16
Misc :
ALS Vial : 51 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AG8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

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

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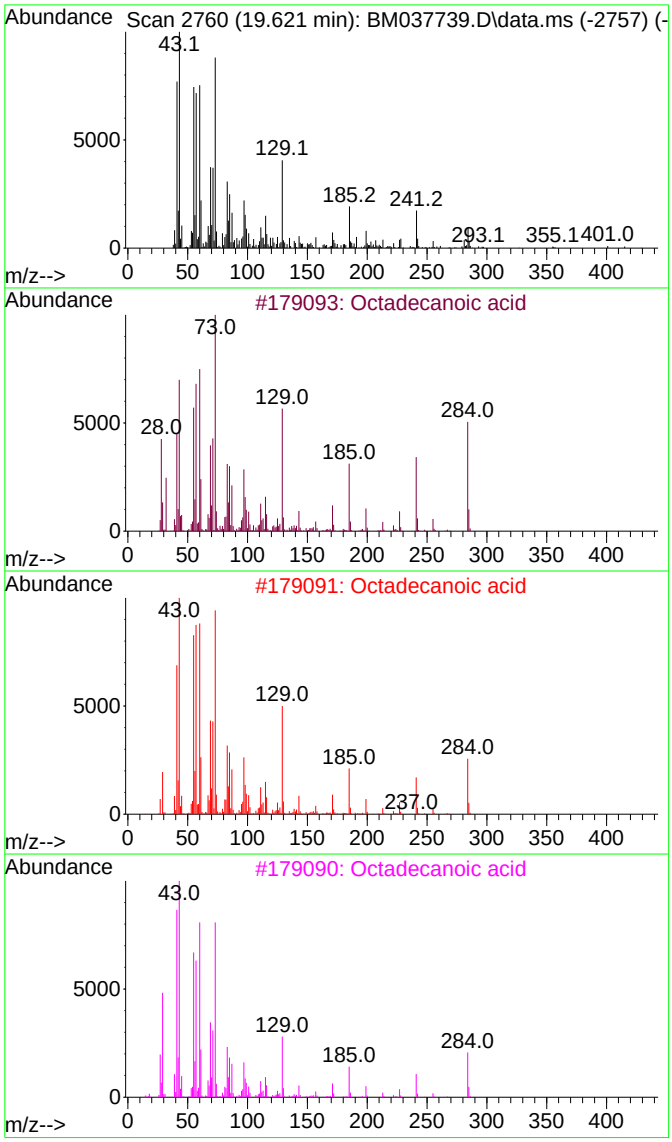
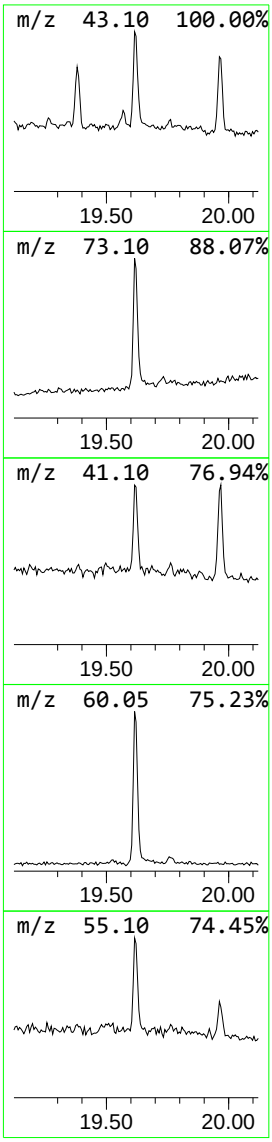
Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.621	2.99 ng/ul	560694	Chrysene-d12	21.639

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	99
3	Octadecanoic acid	284	C18H36O2	000057-11-4	99
4	Octadecanoic acid	284	C18H36O2	000057-11-4	99
5	Octadecanoic acid	284	C18H36O2	000057-11-4	94





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Data File : BM037739.D
Acq On : 26 Nov 2022 18:43
Operator : CG/JU
Sample : N5602-16
Misc :
ALS Vial : 51 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AG8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

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

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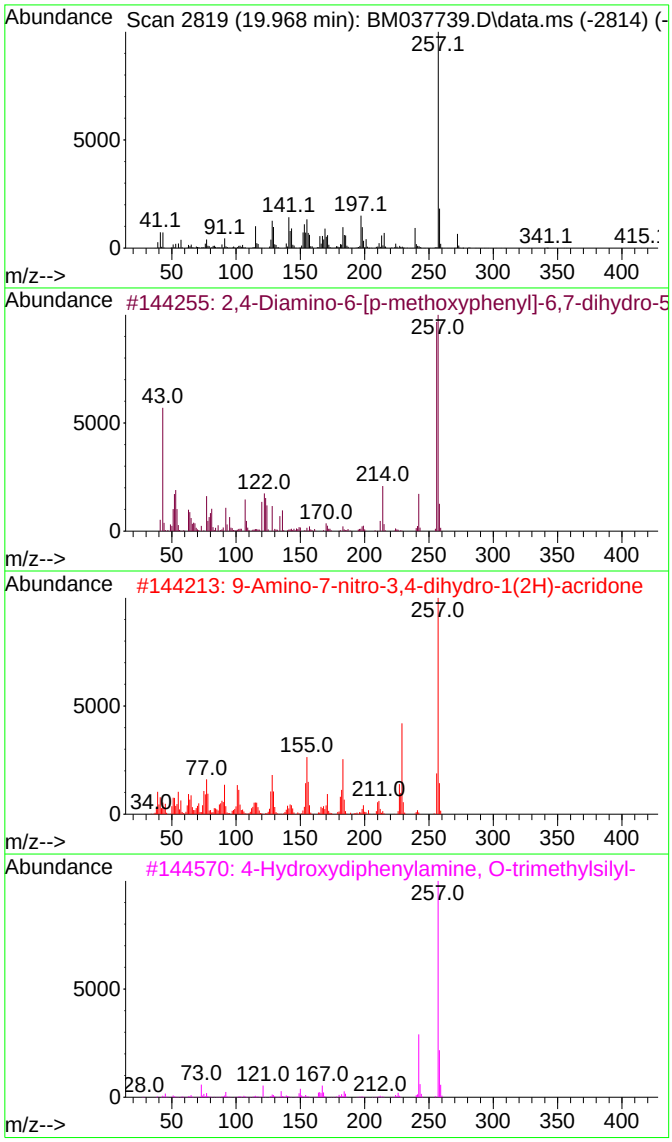
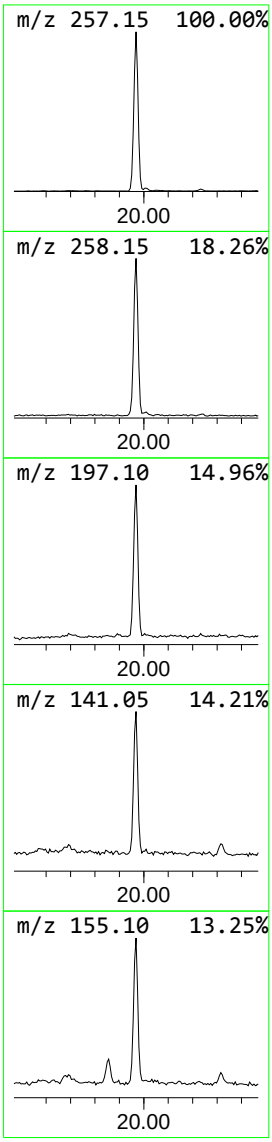
Peak Number 7 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.968	14.37 ng/ul	2693910	Chrysene-d12	21.639

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Diamino-6-[p-methoxyphenyl]-...	257	C13H15N5O	1000251-46-9	49
2	9-Amino-7-nitro-3,4-dihydro-1(2H...	257	C13H11N3O3	104675-31-2	47
3	4-Hydroxydiphenylamine, O-trimet...	257	C15H19NOSi	1000417-42-0	47
4	Benzo[f]quinoline, 5,6-dihydro-3...	257	C19H15N	022877-22-1	46
5	N-allylnormetazocine	257	C17H23NO	014198-28-8	46





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037739.D
Acq On : 26 Nov 2022 18:43
Operator : CG/JU
Sample : N5602-16
Misc :
ALS Vial : 51 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AG8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.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
2-Pentanone, 4-...	5.169	3.8	ng/ul	269800	1	8.110	1421190	20.0
Phenol, p-tert-...	12.257	3.5	ng/ul	397097	2	10.934	2258800	20.0
m-Chlorophenyla...	14.004	15.8	ng/ul	2590220	3	14.733	3281450	20.0
3-tert-Butylben...	14.539	3.0	ng/ul	485538	3	14.733	3281450	20.0
n-Hexadecanoic ...	18.357	3.0	ng/ul	587956	4	17.474	3922660	20.0
Octadecanoic acid	19.621	3.0	ng/ul	560694	5	21.639	3749850	20.0
unknown-01	19.968	14.4	ng/ul	2693910	5	21.639	3749850	20.0