LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111723\
Data File : BP018241.D
Acq On : 18 Nov 2023 03:04
Operator : MA/JU
Sample : 05369-12
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCDN9

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-BP111023.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BP018241.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.158	10	12	18	rVB	17889	21868	0.65%	0.082%
2	3.428	55	58	64	rVB8	4545	6994	0.21%	0.026%
3	3.605	85	88	101	rBV	43221	84223	2.49%	0.314%
4	3.775	111	117	121	rVB5	5174	10649	0.31%	0.040%
5	3.899	135	138	145	rVB7	5586	10117	0.30%	0.038%
6	4.411	220	225	231	rBV4	19368	30560	0.90%	0.114%
7	6.964	654	659	675	rBV	43244	108150	3.19%	0.404%
8	7.128	682	687	702	rBV	244399	405044	11.96%	1.511%
9	7.305	710	717	735	rBV	238069	458001	13.53%	1.709%
10	7.775	791	797	816	rBV	293680	526305	15.54%	1.964%
11	8.510	916	922	941	rBV	144210	315461	9.32%	1.177%
12	8.987	996	1003	1020	rBV	309240	579576	17.12%	2.163%
13	9.152	1026	1031	1036	rVB3	7123	11892	0.35%	0.044%
14	9.387	1066	1071	1080	rBV3	3710	10420	0.31%	0.039%
15	9.699	1118	1124	1139	rBV	277791	518776	15.32%	1.936%
16	9.975	1165	1171	1172	rBV6	4121	8139	0.24%	0.030%
17	10.228	1208	1214	1235	rBV	292269	672212	19.85%	2.508%
18	10.593	1269	1276	1288	rBV	407621	690268	20.38%	2.576%
19	10.787	1302	1309	1330	rBV	168720	423467	12.51%	1.580%
20	10.981	1337	1342	1351	rVB	6724	17308	0.51%	0.065%
21	11.140	1363	1369	1370	rBV6	4471	7314	0.22%	0.027%
22	11.404	1404	1414	1424	rVV5	16787	61652	1.82%	0.230%
23	11.481	1424	1427	1431	rVV6	9820	21238	0.63%	0.079%
24	11.522	1432	1434	1440	rVV6	9903	18910	0.56%	0.071%
25	11.563	1440	1441	1447	rVB6	4143	4581	0.14%	0.017%
26	11.646	1451	1455	1459	rVB6	4282	6109	0.18%	0.023%
27	12.216	1547	1552	1560	rVB9	6617	14577	0.43%	0.054%
28	12.740	1636	1641	1647	rVB9	2745	5987	0.18%	0.022%
29	12.910	1665	1670	1679	rBV9	6934	17645	0.52%	0.066%
30	13.298	1728	1736	1742	rBV2	35154	59592	1.76%	0.222%
31	13.422	1752	1757	1764	rBV9	2165	5074	0.15%	0.019%
32	13.663	1793	1798	1809	rVB9	9655	17182	0.51%	0.064%
33	13.781	1811	1818	1829	rBV3	13511	53063	1.57%	0.198%
34	13.881	1829	1835	1848	rVB	1053220	1407595	41.57%	5.252%
35	14.157	1874	1882	1899	rBV	943652	1375828	40.63%	5.134%
36	14.316	1904	1909	1913	rVB8	5292	11229	0.33%	0.042%

LSC Area Percent Report

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Data File : BP018241.D
Acq On : 18 Nov 2023 03:04
Operator : MA/JU
Sample : 05369-12
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCDN9

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-BP111023.MA.M
Title : SVOA CALIBRATION

37	14.457	1926	1933	1942	rBV	677299	970607	28.66%	3.622%
38	14.545	1944	1948	1952	rBV5	8679	14378	0.42%	0.054%
39	14.716	1970	1977	1981	rBV10	2797	5789	0.17%	0.022%
40	14.787	1981	1989	1996	rBV6	21650	75676	2.23%	0.282%
41	14.857	1999	2001	2012	rVV10	15204	37898	1.12%	0.141%
42	14.963	2014	2019	2024	rVB9	2009	4912	0.15%	0.018%
43	15.098	2036	2042	2046	rBV8	3818	6071	0.18%	0.023%
44	15.240	2062	2066	2069	rBV5	3397	5532	0.16%	0.021%
45	15.463	2097	2104	2112	rBV	1370948	1884021	55.64%	7.030%
46	15.528	2112	2115	2117	rVV3	8033	10064	0.30%	0.038%
47	15.563	2117	2121	2126	rVB	39276	54108	1.60%	0.202%
48	15.622	2126	2131	2143	rBV	458810	747304	22.07%	2.788%
49	15.875	2169	2174	2178	rBV	17101	26639	0.79%	0.099%
50	15.922	2178	2182	2186	rVV3	8093	11478	0.34%	0.043%
51	16.057	2200	2205	2210	rBV8	4851	9577	0.28%	0.036%
52	16.181	2220	2226	2232	rBV	39184	55571	1.64%	0.207%
53	16.275	2235	2242	2246	rVV	101300	145003	4.28%	0.541%
54	16.334	2246	2252	2258	rVV3	174754	309674	9.14%	1.155%
55	16.392	2258	2262	2266	rVV2	102632	173257	5.12%	0.646%
56	16.439	2266	2270	2275	rVV	69268	103398	3.05%	0.386%
57	16.492	2275	2279	2281	rVV	36705	57003	1.68%	0.213%
58	16.539	2285	2287	2291	rVV2	38033	46251	1.37%	0.173%
59	16.598	2291	2297	2304	rVV3	101148	197193	5.82%	0.736%
60	16.669	2304	2309	2314	rVV	94639	157367	4.65%	0.587%
61	16.704	2314	2315	2318	rVV3	29019	34896	1.03%	0.130%
62	16.739	2318	2321	2329	rVB	53428	75643	2.23%	0.282%
63	16.875	2341	2344	2347	rBV5	5579	8196	0.24%	0.031%
64	16.916	2347	2351	2354	rVB5	5961	7805	0.23%	0.029%
65	16.951	2354	2357	2358	rBV3	4472	3920	0.12%	0.015%
66	17.045	2368	2373	2375	rBV5	4287	6620	0.20%	0.025%
67	17.104	2381	2383	2390	rVB7	3082	4469	0.13%	0.017%
68	17.239	2400	2406	2417	rVV	956209	1283892	37.91%	4.791%
69	17.339	2417	2423	2442	rVV	1530194	2228325	65.80%	8.315%
70	17.498	2445	2450	2456	rVV8	7569	19886	0.59%	0.074%
71	17.575	2460	2463	2467	rVB5	6120	7962	0.24%	0.030%
72	17.875	2510	2514	2518	rBV6	18321	23875	0.71%	0.089%
73	18.092	2547	2551	2559	rBV2	74696	108688	3.21%	0.406%
74	18.186	2564	2567	2572	rVB	9389	12363	0.37%	0.046%
75	18.304	2583	2587	2592	rBV	116460	157743	4.66%	0.589%
76	19.169	2731	2734	2737	rBV3	18233	24205	0.71%	0.090%

LSC Area Percent Report

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Acq On : 18 Nov 2023 03:04
Operator : MA/JU
Sample : 05369-12
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCDN9

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-BP111023.MA.M
Title : SVOA CALIBRATION

77	19.245	2745	2747	2751	rVB	20085	25183	0.74%	0.094%
78	19.339	2759	2763	2769	rBV	62528	87669	2.59%	0.327%
79	19.598	2801	2807	2817	rBV	2221520	2872042	84.81%	10.716%
80	21.375	3104	3109	3118	rBV	1229139	1553590	45.88%	5.797%
81	23.680	3494	3501	3514	rVB2	1763877	3386315	100.00%	12.635%
82	23.845	3522	3529	3542	rVB	840054	1761281	52.01%	6.572%

Sum of corrected areas: 26800345

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111723\
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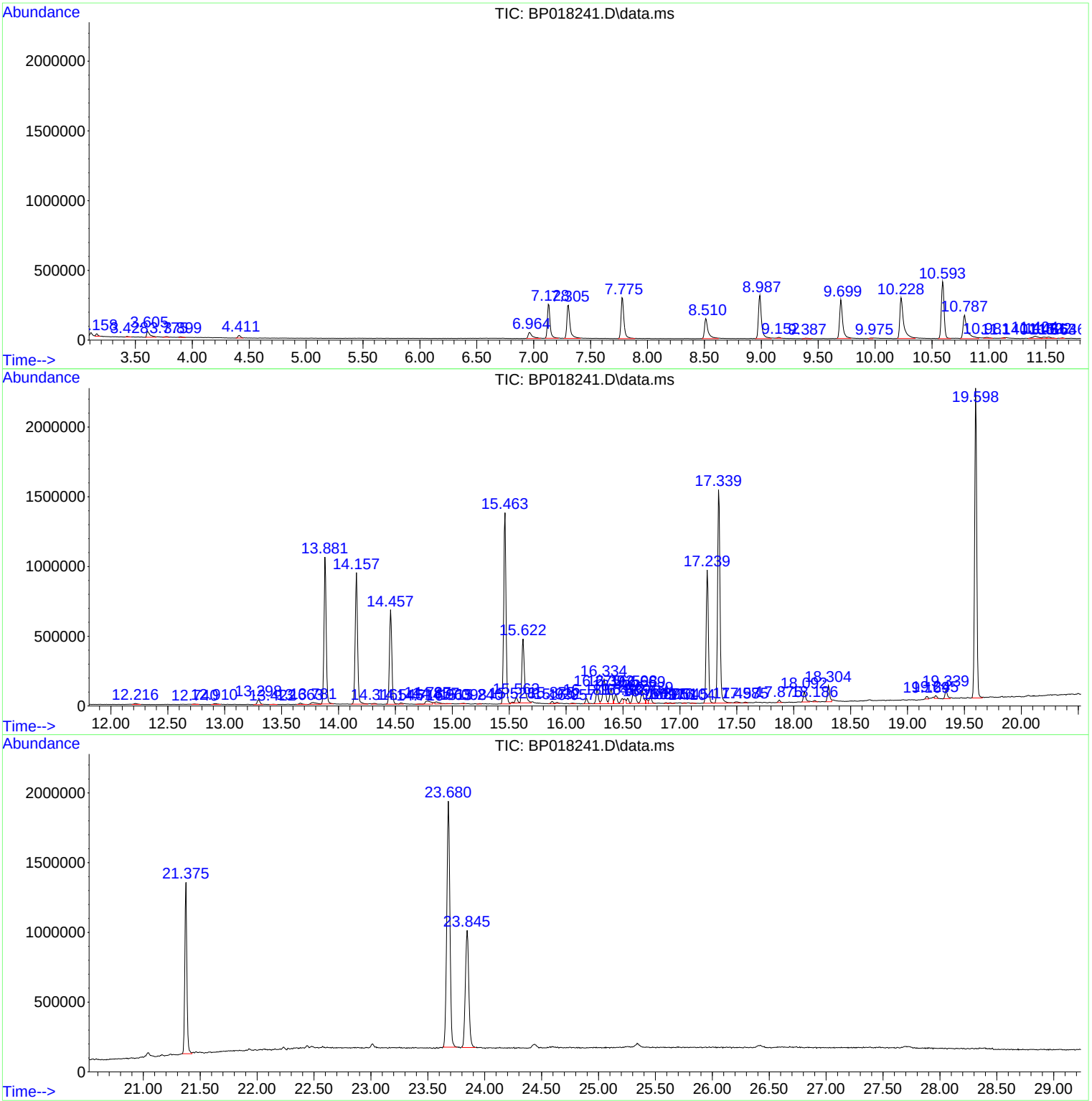
Instrument :
BNA_P
ClientSampleId :
GCDN9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111723\
Data File : BP018241.D
Acq On : 18 Nov 2023 03:04
Operator : MA/JU
Sample : 05369-12
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCDN9

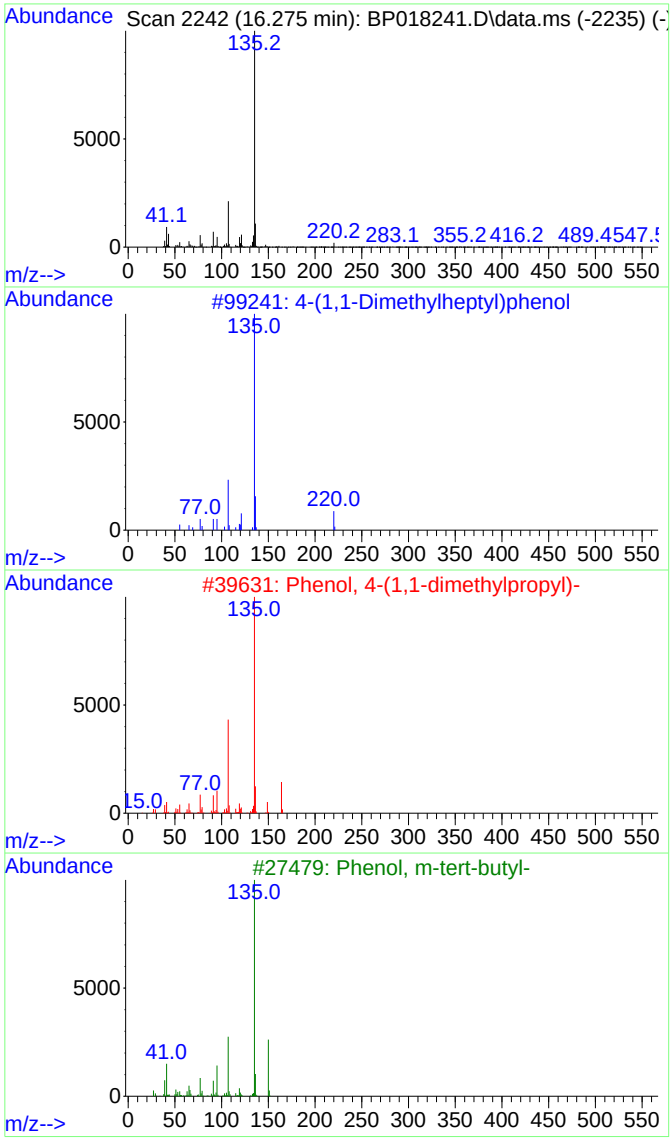
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

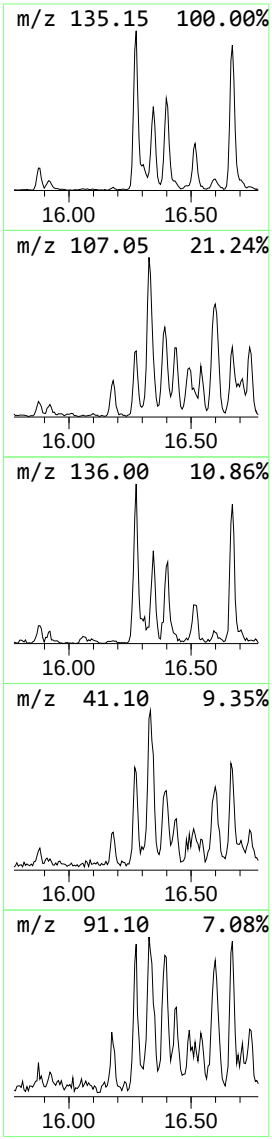
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 4-(1,1-Dimethylheptyl)phenol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.275	2.26 ng/ul	145003	Phenanthrene-d10	17.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(1,1-Dimethylheptyl)phenol	220	C15H24O	1000384-80-3	90
2	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	78
3	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	78
4	Hexestrol, O-pentafluoropropionyl-	416	C21H21F5O3	1010365-43-4	72
5	Methanol, (cyclohexyl)(2,3-dimet...	218	C15H22O	349498-47-1	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111723\
Data File : BP018241.D
Acq On : 18 Nov 2023 03:04
Operator : MA/JU
Sample : 05369-12
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCDN9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

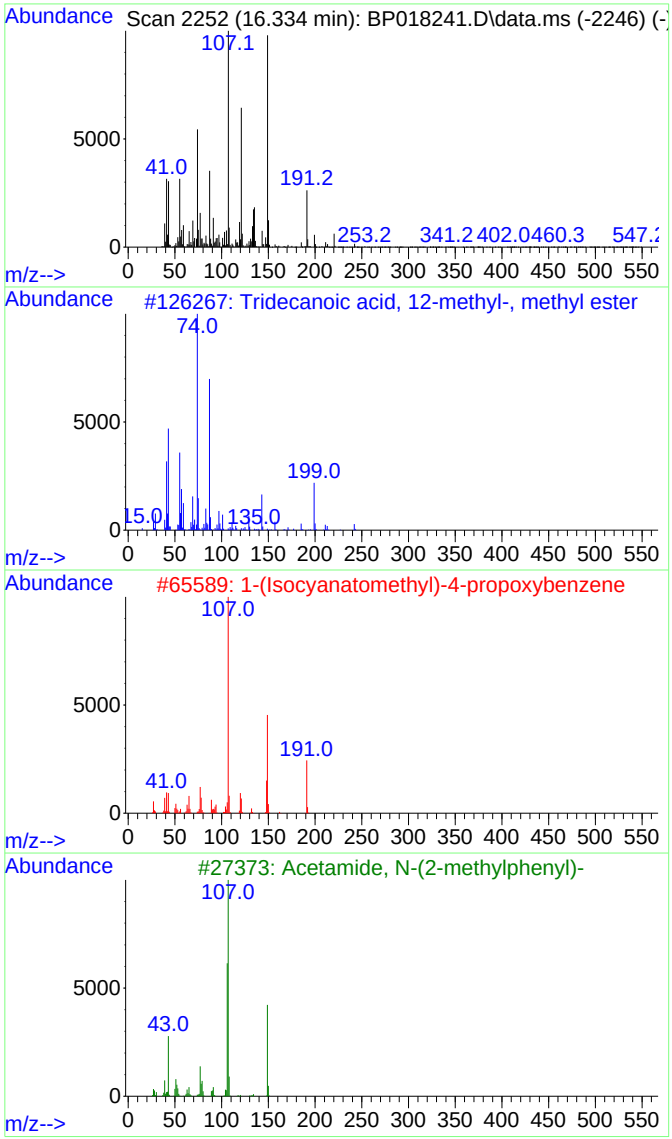
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

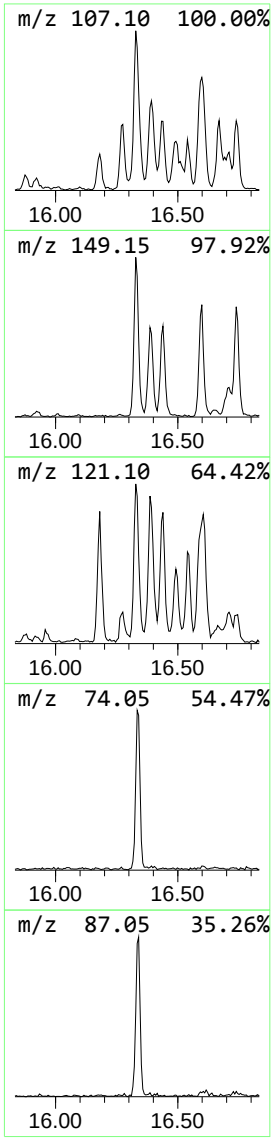
****

Peak Number 2 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.334	4.82 ng/ul	309674	Phenanthrene-d10	17.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	45
2	1-(Isocyanatomethyl)-4-propoxybe...	191	C11H13NO2	936095-07-7	43
3	Acetamide, N-(2-methylphenyl)-	149	C9H11NO	000120-66-1	38
4	Acetamide, N-(4-methylphenyl)-	149	C9H11NO	000103-89-9	27
5	Butanamide, N-(4-methylphenyl)-3...	191	C11H13NO2	002415-85-2	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111723\
Data File : BP018241.D
Acq On : 18 Nov 2023 03:04
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Sample : 05369-12
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCDN9

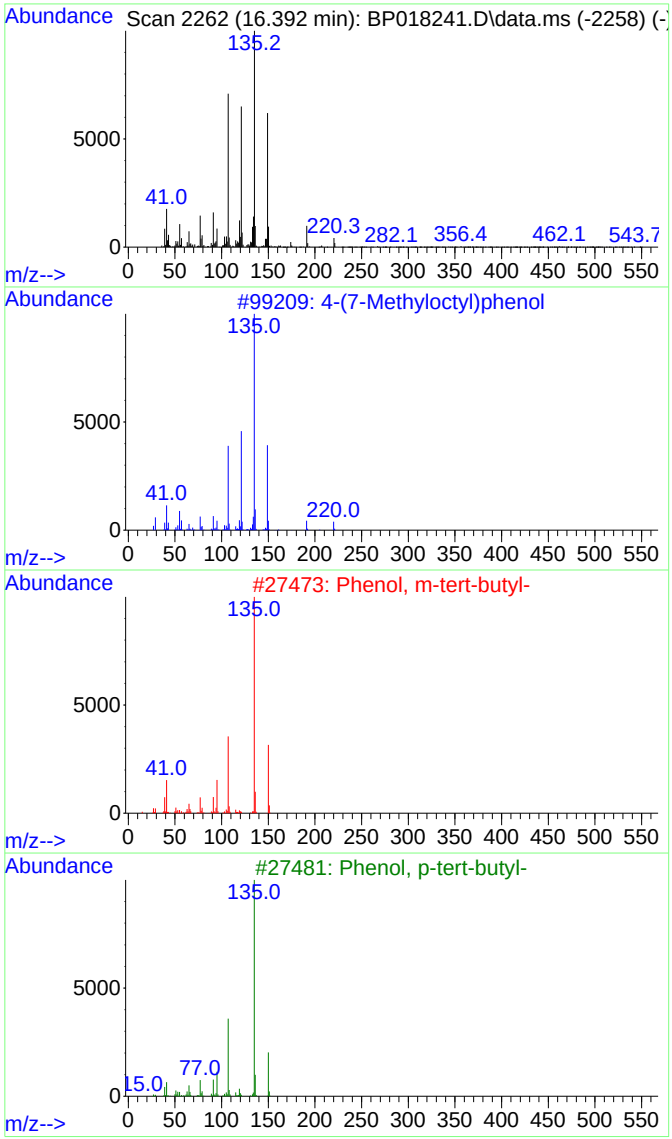
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

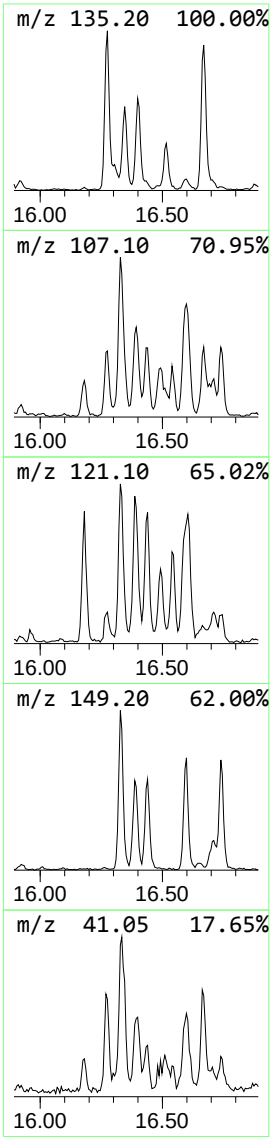
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.392	2.70 ng/ul	173257	Phenanthrene-d10	17.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(7-Methyloctyl)phenol	220	C15H24O	024518-48-7	86
2	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	49
3	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	49
4	Hexestrol	270	C18H22O2	000084-16-2	47
5	Benzaldehyde diethylacetal	180	C11H16O2	000774-48-1	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111723\
Data File : BP018241.D
Acq On : 18 Nov 2023 03:04
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Sample : 05369-12
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCDN9

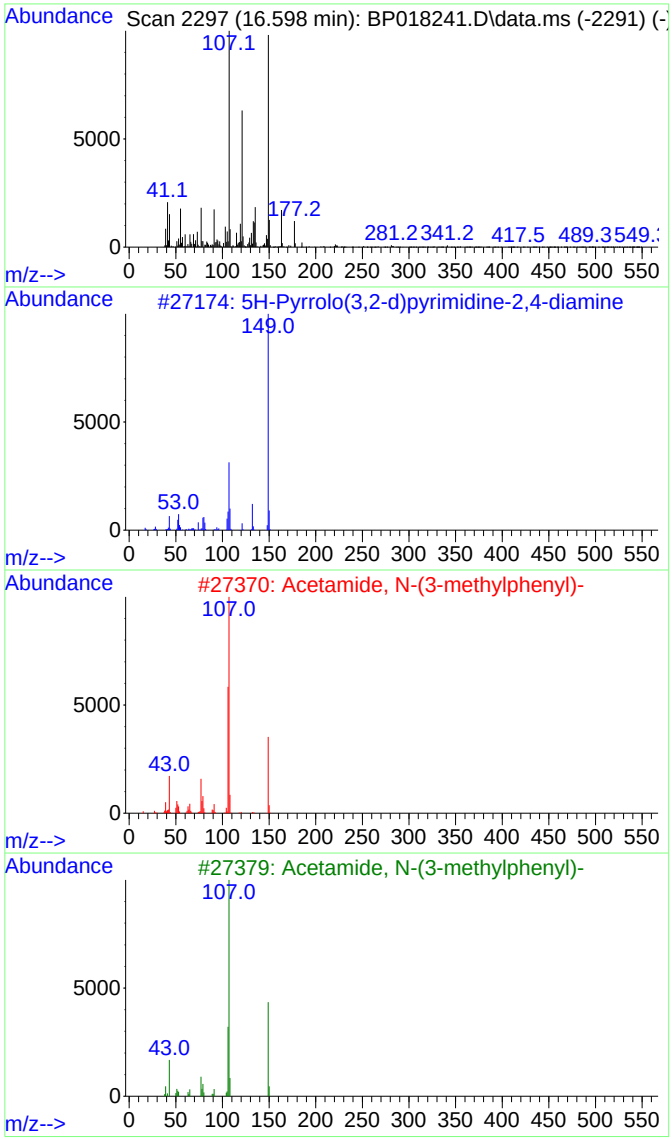
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

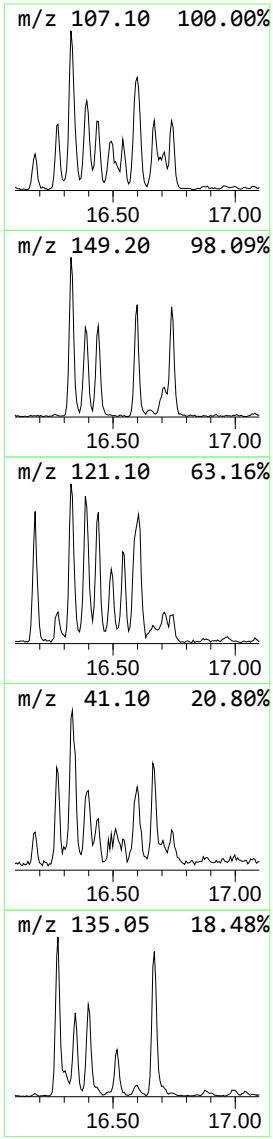
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 5H-Pyrrolo(3,2-d)pyrimidine... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.598	3.07 ng/ul	197193	Phenanthrene-d10	17.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-Pyrrolo(3,2-d)pyrimidine-2,4-...	149	C6H7N5	1000244-21-4	59
2	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	58
3	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	53
4	Acetic acid, (2-bromophenyl)meth...	228	C9H9BrO2	1000368-71-4	53
5	1-(1,3-Benzodioxol-5-yl)-2-hydro...	298	C17H14O5	1000510-10-3	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111723\
Data File : BP018241.D
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Sample : 05369-12
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCDN9

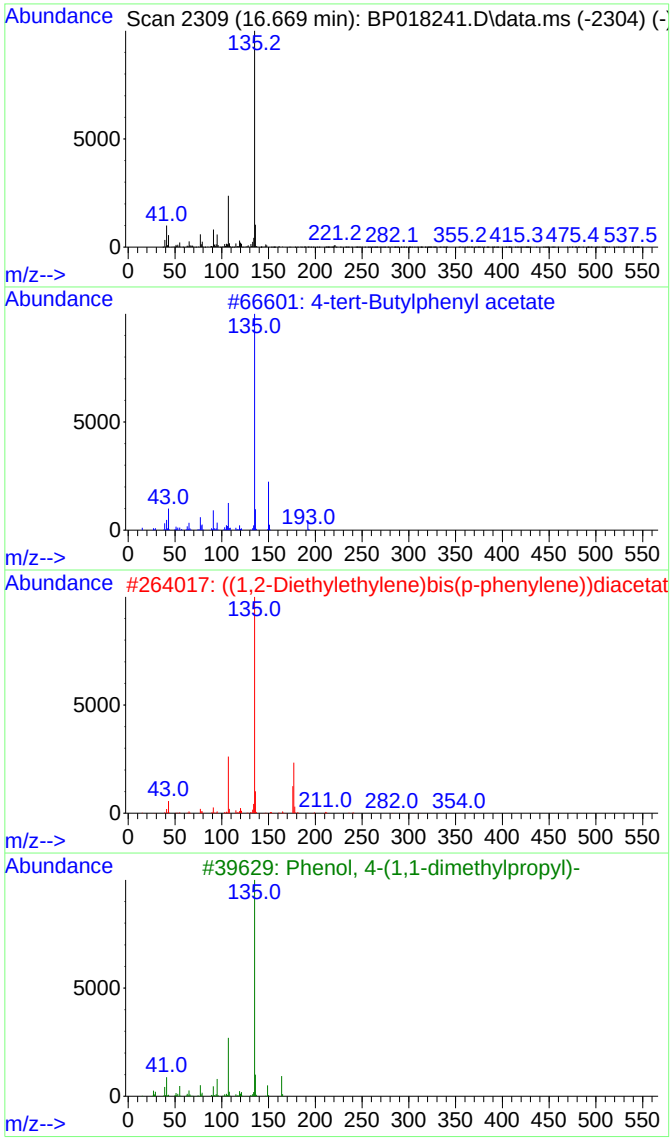
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

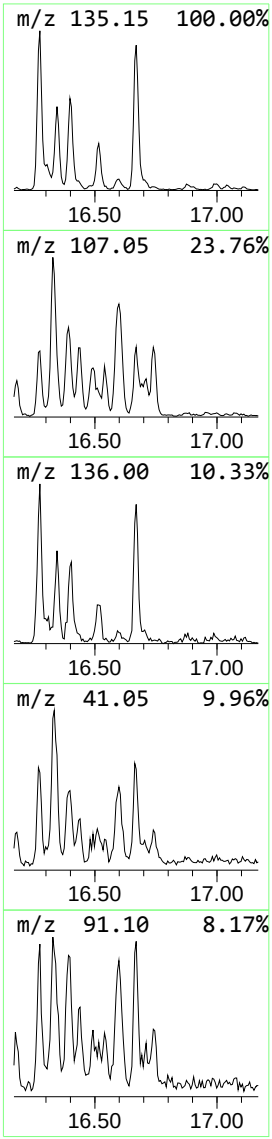
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4-tert-Butylphenyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.669	2.45 ng/ul	157367	Phenanthrene-d10	17.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-tert-Butylphenyl acetate	192	C12H16O2	003056-64-2	78
2	((1,2-Diethylethylene)bis(p-phen...	354	C22H26O4	004547-76-6	78
3	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	78
4	4-(1,1-Dimethylpropyl)phenyl ace...	206	C13H18O2	1000373-45-3	72
5	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111723\
Data File : BP018241.D
Acq On : 18 Nov 2023 03:04
Operator : MA/JU
Sample : 05369-12
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCDN9

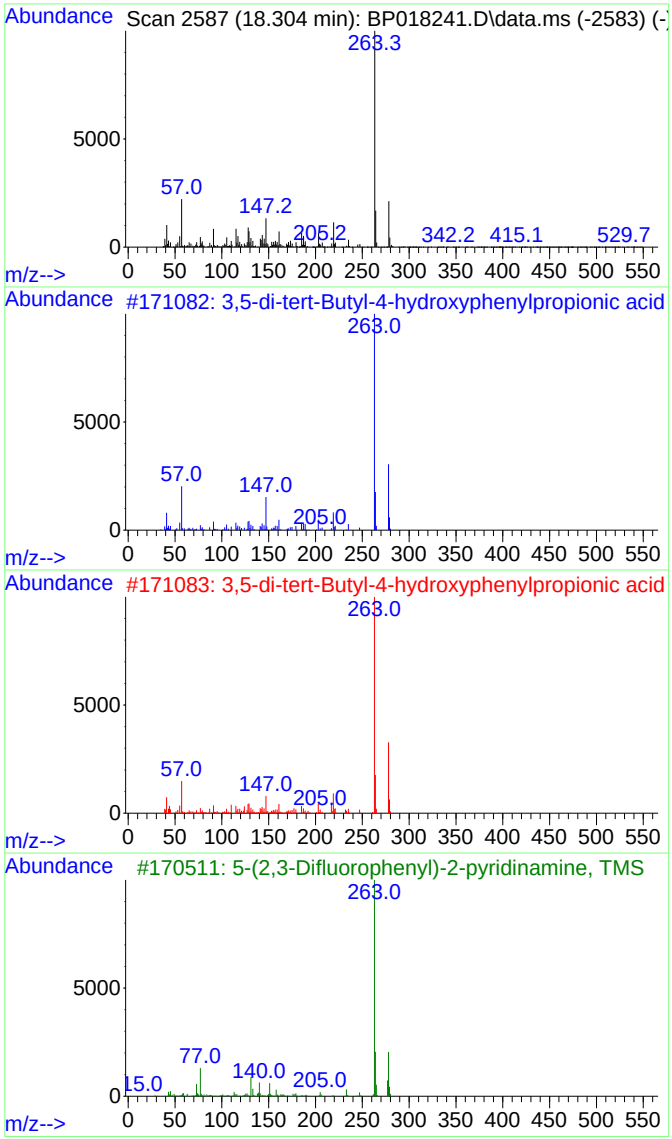
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

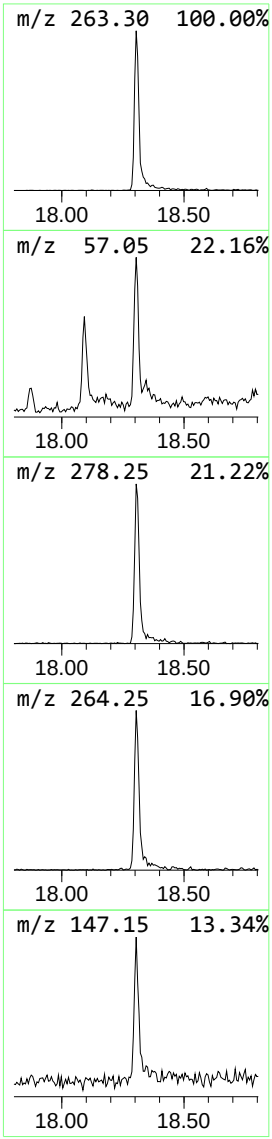
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 3,5-di-tert-Butyl-4-hydroxy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.304	2.46 ng/ul	157743	Phenanthrene-d10	17.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-di-tert-Butyl-4-hydroxypheny...	278	C17H26O3	020170-32-5	96
2	3,5-di-tert-Butyl-4-hydroxypheny...	278	C17H26O3	020170-32-5	91
3	5-(2,3-Difluorophenyl)-2-pyridin...	278	C14H16F2N2Si	1000504-49-4	76
4	Cyanic acid, (1-methylethylidene...	278	C17H14N2O2	001156-51-0	64
5	6,7-Dimethoxy-4(1H)-quinazolinon...	278	C13H18N2O3Si	1000479-65-5	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111723\
Data File : BP018241.D
Acq On : 18 Nov 2023 03:04
Operator : MA/JU
Sample : 05369-12
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCDN9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.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
4-(1,1-Dimethyl...	16.275	2.3	ng/ul	145003	4	17.239	1283890	20.0
unknown-01	16.334	4.8	ng/ul	309674	4	17.239	1283890	20.0
4-(7-Methylocty...	16.392	2.7	ng/ul	173257	4	17.239	1283890	20.0
5H-Pyrrolo(3,2-...	16.598	3.1	ng/ul	197193	4	17.239	1283890	20.0
4-tert-Butylphe...	16.669	2.5	ng/ul	157367	4	17.239	1283890	20.0
3,5-di-tert-But...	18.304	2.5	ng/ul	157743	4	17.239	1283890	20.0