

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111723\
 Data File : BP018256.D
 Acq On : 18 Nov 2023 12:07
 Operator : MA/JU
 Sample : 05370-08
 Misc :
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 GCDQ4

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: BP018256.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	9	12	17	rVB	12165	15674	0.73%	0.083%
2	3.605	85	88	101	rBV	42925	88622	4.12%	0.471%
3	3.770	114	116	120	rVB5	5163	6181	0.29%	0.033%
4	3.899	136	138	143	rVB4	3800	3185	0.15%	0.017%
5	4.346	210	214	216	rBV5	1980	2517	0.12%	0.013%
6	4.458	231	233	237	rVB5	2009	2495	0.12%	0.013%
7	4.823	293	295	299	rBV5	1682	2195	0.10%	0.012%
8	6.593	592	596	599	rBV6	1680	2539	0.12%	0.013%
9	6.964	654	659	673	rBV	42555	103753	4.82%	0.551%
10	7.128	682	687	703	rVB	210196	344549	16.00%	1.830%
11	7.299	710	716	739	rBV	223909	419523	19.49%	2.228%
12	7.781	791	798	810	rBV	183317	340978	15.84%	1.811%
13	8.511	916	922	941	rBV	144841	303984	14.12%	1.614%
14	8.987	996	1003	1020	rBV	248701	492306	22.87%	2.614%
15	9.699	1115	1124	1144	rBV	218566	438483	20.37%	2.328%
16	10.140	1195	1199	1204	rBV8	1924	4044	0.19%	0.021%
17	10.228	1207	1214	1237	rVV	242461	558095	25.92%	2.964%
18	10.375	1237	1239	1243	rVV5	5069	8116	0.38%	0.043%
19	10.434	1247	1249	1252	rVB3	2659	2234	0.10%	0.012%
20	10.593	1270	1276	1285	rBV	257399	443685	20.61%	2.356%
21	10.781	1302	1308	1328	rBV	173085	441518	20.51%	2.345%
22	10.981	1340	1342	1346	rBV5	2560	3073	0.14%	0.016%
23	11.157	1368	1372	1374	rVV5	2711	3942	0.18%	0.021%
24	11.399	1404	1413	1423	rBV5	5879	18739	0.87%	0.100%
25	12.240	1550	1556	1557	rBV6	3735	4671	0.22%	0.025%
26	12.628	1619	1622	1627	rBV7	1659	2830	0.13%	0.015%
27	13.299	1729	1736	1744	rBV	113870	187663	8.72%	0.997%
28	13.663	1794	1798	1802	rBV7	2093	3400	0.16%	0.018%
29	13.881	1829	1835	1852	rBV	665744	980529	45.55%	5.207%
30	14.157	1875	1882	1895	rBV	695690	1013035	47.06%	5.380%
31	14.287	1901	1904	1909	rVV7	3281	3911	0.18%	0.021%
32	14.334	1909	1912	1916	rVB6	2179	2230	0.10%	0.012%
33	14.457	1927	1933	1943	rBV	394309	577736	26.84%	3.068%
34	14.716	1971	1977	1980	rBV8	1884	3259	0.15%	0.017%
35	14.804	1985	1992	1998	rBV7	12142	34014	1.58%	0.181%
36	14.969	2016	2020	2026	rVB8	2675	5825	0.27%	0.031%

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111723\
 Data File : BP018256.D
 Acq On : 18 Nov 2023 12:07
 Operator : MA/JU
 Sample : 05370-08
 Misc :
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 GCDQ4

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	15.463	2095	2104	2113	rBV	901070	1332340	61.89%	7.075%
38	15.628	2126	2132	2144	rBV	267176	476045	22.11%	2.528%
39	15.710	2144	2146	2155	rVV8	11853	23789	1.11%	0.126%
40	15.769	2155	2156	2161	rVB5	2838	3394	0.16%	0.018%
41	15.881	2170	2175	2178	rBV	14744	21001	0.98%	0.112%
42	15.922	2178	2182	2186	rVV3	12485	18237	0.85%	0.097%
43	15.963	2186	2189	2194	rVB7	4198	6086	0.28%	0.032%
44	16.181	2222	2226	2232	rBV	29539	38808	1.80%	0.206%
45	16.275	2236	2242	2246	rVV	92576	125132	5.81%	0.664%
46	16.334	2247	2252	2258	rVV2	110515	212213	9.86%	1.127%
47	16.398	2258	2263	2267	rVV2	88933	159718	7.42%	0.848%
48	16.440	2267	2270	2275	rVV	57489	79405	3.69%	0.422%
49	16.498	2275	2280	2281	rVV2	34020	49457	2.30%	0.263%
50	16.516	2281	2283	2285	rVV	30047	35805	1.66%	0.190%
51	16.545	2285	2288	2291	rVV	32131	42259	1.96%	0.224%
52	16.598	2291	2297	2304	rVV3	74563	153828	7.15%	0.817%
53	16.669	2304	2309	2314	rVV	88247	139084	6.46%	0.739%
54	16.710	2314	2316	2318	rVV2	25067	30095	1.40%	0.160%
55	16.740	2318	2321	2329	rVB	39506	60556	2.81%	0.322%
56	16.875	2340	2344	2349	rBV8	3262	6933	0.32%	0.037%
57	16.945	2355	2356	2358	rBV2	2386	2484	0.12%	0.013%
58	17.040	2370	2372	2375	rBV4	2646	2826	0.13%	0.015%
59	17.075	2377	2378	2383	rVB5	3097	3139	0.15%	0.017%
60	17.240	2398	2406	2418	rBV	549873	791059	36.75%	4.201%
61	17.345	2418	2424	2441	rVV	1165405	1719122	79.86%	9.129%
62	17.498	2446	2450	2457	rVB9	5034	10238	0.48%	0.054%
63	17.692	2478	2483	2484	rBV5	2332	3364	0.16%	0.018%
64	17.875	2509	2514	2522	rBV9	15859	23538	1.09%	0.125%
65	18.098	2547	2552	2562	rVV2	40882	67478	3.13%	0.358%
66	18.192	2565	2568	2571	rVV4	3357	4675	0.22%	0.025%
67	18.304	2583	2587	2594	rBV	72491	107674	5.00%	0.572%
68	18.986	2700	2703	2705	rBV4	4522	5687	0.26%	0.030%
69	19.016	2705	2708	2712	rVB4	21028	23059	1.07%	0.122%
70	19.169	2731	2734	2739	rBV3	14028	18702	0.87%	0.099%
71	19.251	2742	2748	2755	rVB3	14167	30668	1.42%	0.163%
72	19.345	2760	2764	2770	rBV5	28462	43879	2.04%	0.233%
73	19.604	2802	2808	2818	rBV	1675751	2152772	100.00%	11.432%
74	21.039	3049	3052	3061	rBV10	21528	45899	2.13%	0.244%
75	21.380	3105	3110	3122	rBV	643243	894873	41.57%	4.752%
76	23.686	3495	3502	3516	rVB2	1076723	2101418	97.61%	11.159%

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111723\
Data File : BP018256.D
Acq On : 18 Nov 2023 12:07
Operator : MA/JU
Sample : 05370-08
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCDQ4

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	23.857	3524	3531	3542	rVB	418590	894995	41.57%	4.753%
----	--------	------	------	------	-----	--------	--------	--------	--------

Sum of corrected areas: 18831267

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111723\
Data File : BP018256.D
Acq On : 18 Nov 2023 12:07
Operator : MA/JU
Sample : 05370-08
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCDQ4

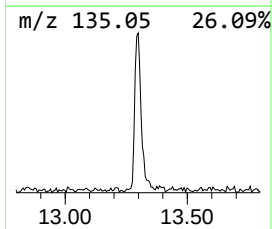
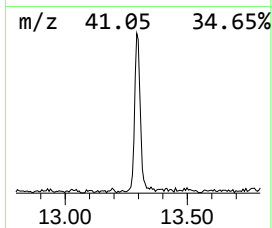
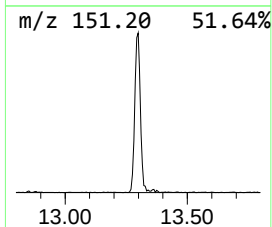
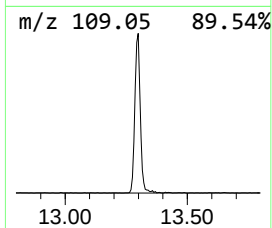
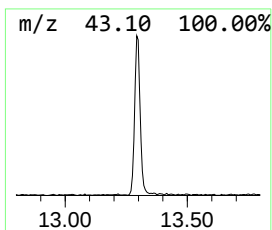
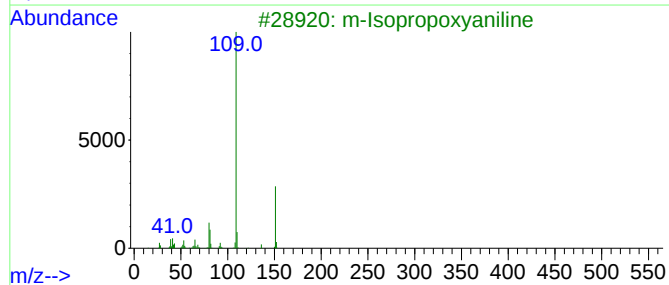
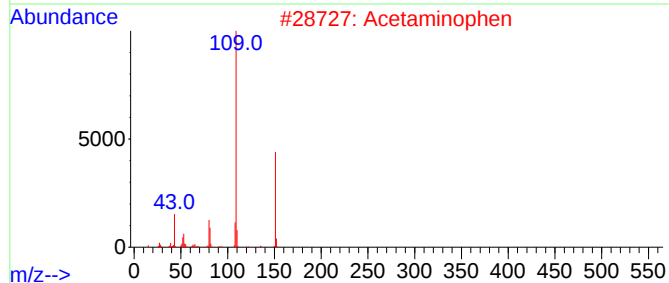
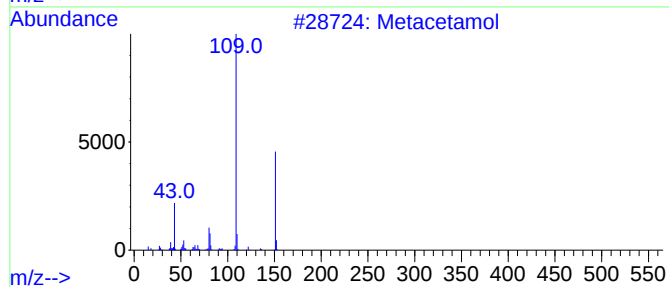
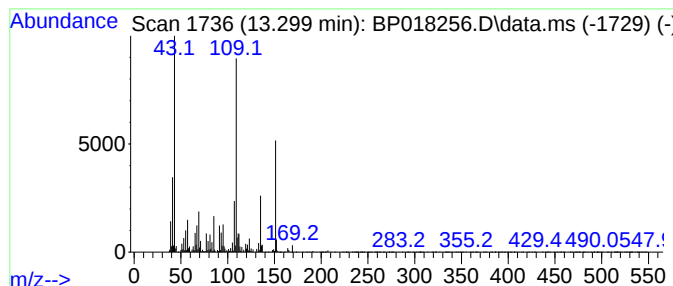
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.299	6.50 ng/ul	187663	Acenaphthene-d10	14.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Metacetamol	151	C8H9NO2	000621-42-1	49
2			Acetaminophen	151	C8H9NO2	000103-90-2	49
3			m-Isopropoxyaniline	151	C9H13NO	041406-00-2	49
4			Metacetamol	151	C8H9NO2	000621-42-1	47
5			Metacetamol	151	C8H9NO2	000621-42-1	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111723\
Data File : BP018256.D
Acq On : 18 Nov 2023 12:07
Operator : MA/JU
Sample : 05370-08
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCDQ4

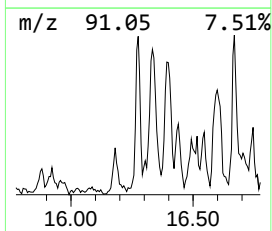
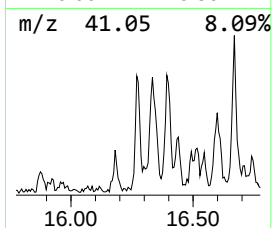
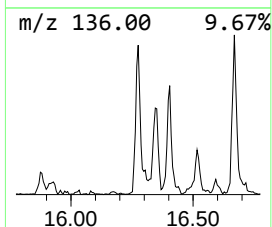
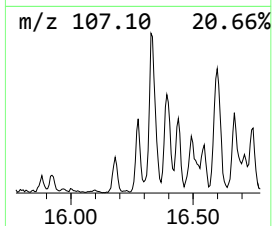
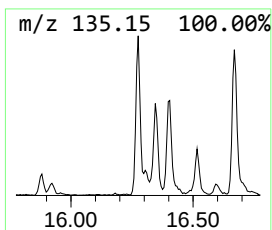
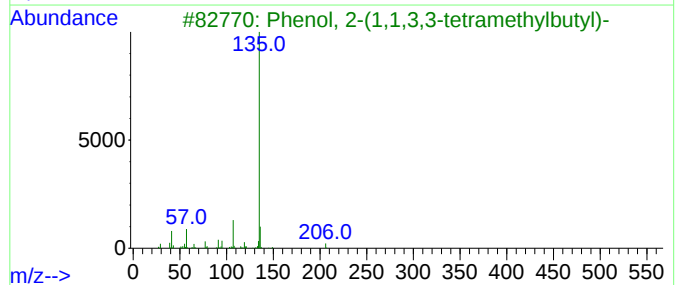
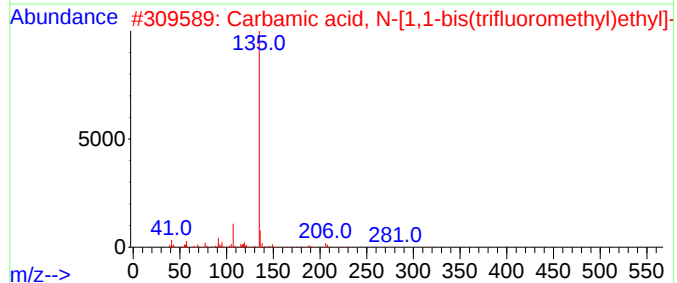
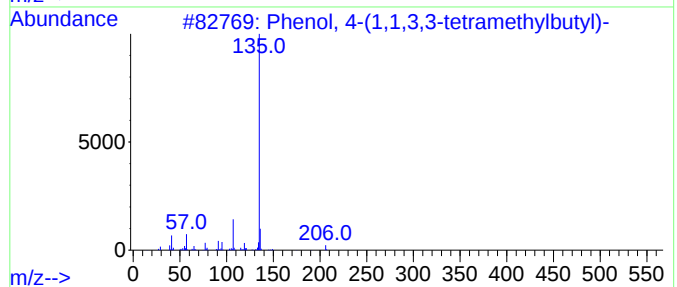
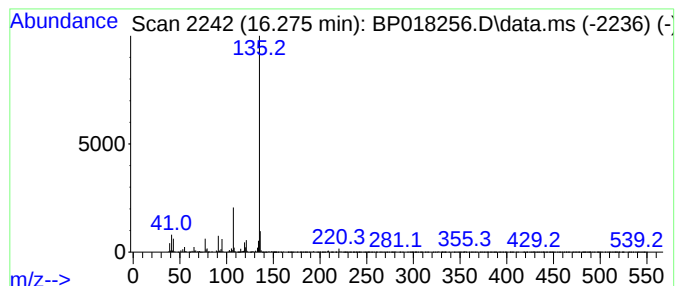
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Phenol, 4-(1,1,3,3-tetramet... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.275	3.16 ng/ul	125132	Phenanthrene-d10	17.240

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	86
2			Carbamic acid, N-[1,1-bis(triflu...	413	C19H25F6NO2	296242-69-8	78
3			Phenol, 2-(1,1,3,3-tetramethylbu...	206	C14H22O	003884-95-5	78
4			Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	78
5			2-tert-Butylphenol, O-(n-propylo...	236	C14H20O3	1000487-37-9	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111723\
Data File : BP018256.D
Acq On : 18 Nov 2023 12:07
Operator : MA/JU
Sample : 05370-08
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCDQ4

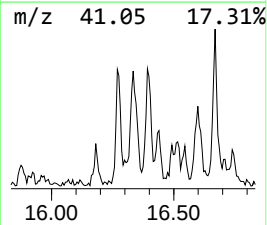
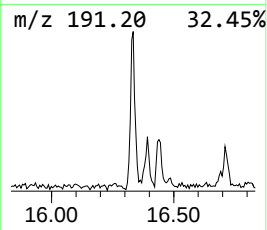
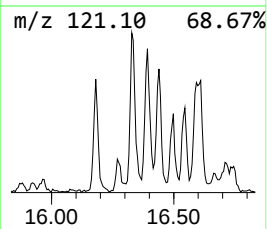
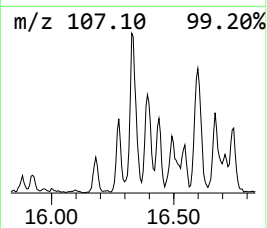
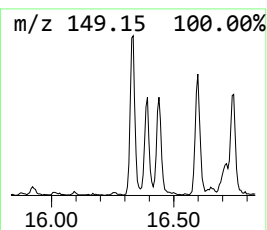
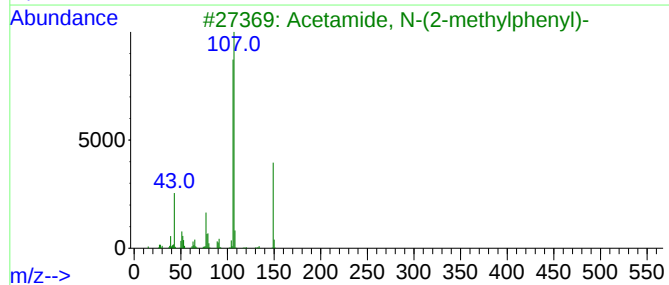
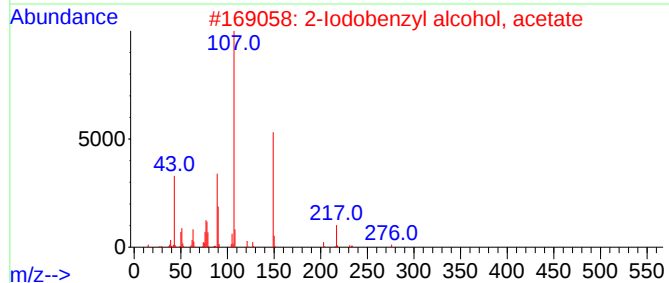
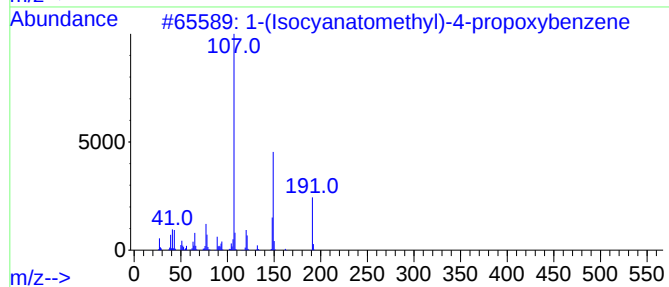
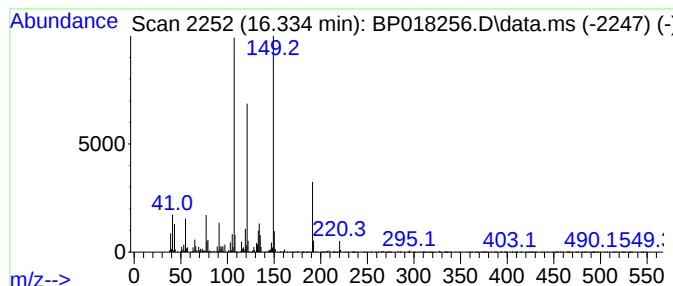
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 1-(Isocyanatomethyl)-4-prop... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.334	5.37 ng/ul	212213	Phenanthrene-d10	17.240

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(Isocyanatomethyl)-4-propoxybe...	191	C11H13NO2	936095-07-7	80		
2	2-Iodobenzyl alcohol, acetate	276	C9H9IO2	1000364-47-1	53		
3	Acetamide, N-(2-methylphenyl)-	149	C9H11NO	000120-66-1	46		
4	Acetamide, N-(2-methylphenyl)-	149	C9H11NO	000120-66-1	46		
5	1-(6-Methyl-2-pyridyl)propan-2-one	149	C9H11NO	065702-08-1	43		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111723\
Data File : BP018256.D
Acq On : 18 Nov 2023 12:07
Operator : MA/JU
Sample : 05370-08
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCDQ4

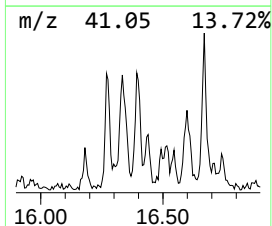
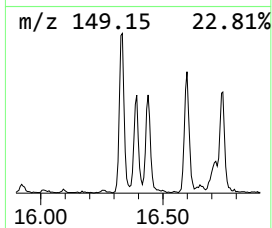
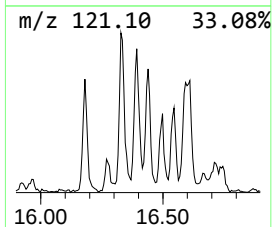
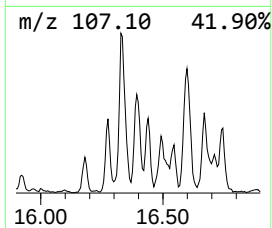
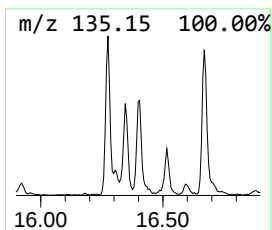
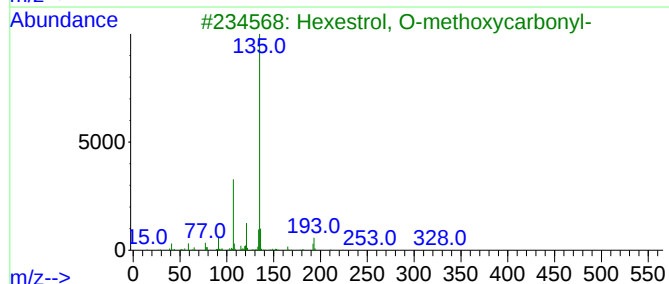
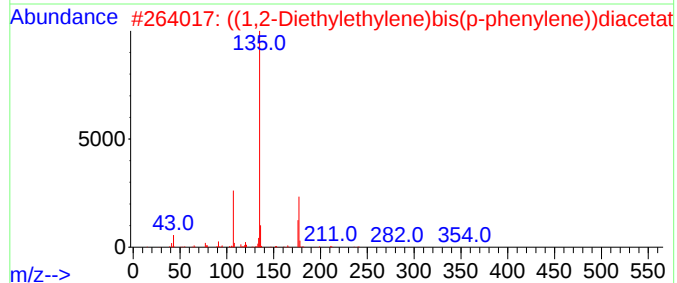
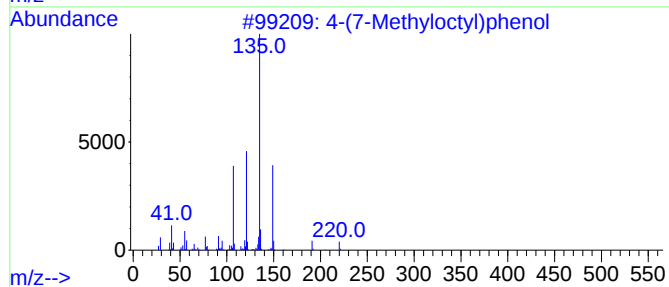
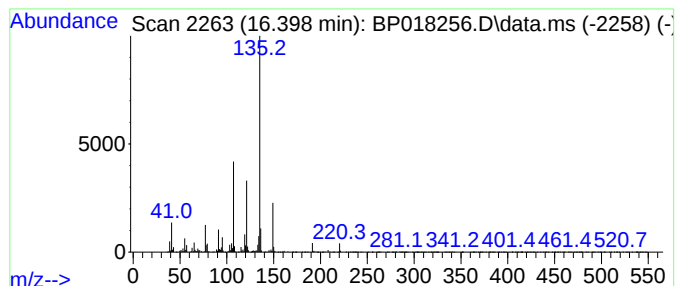
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.398	4.04 ng/ul	159718	Phenanthrene-d10	17.240

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-(7-Methyloctyl)phenol	220	C15H24O	024518-48-7	91
2			((1,2-Diethylethylene)bis(p-phen...	354	C22H26O4	004547-76-6	64
3			Hexestrol, O-methoxycarbonyl-	328	C20H24O4	1000487-66-3	64
4			Hexestrol, O-pentafluoropropionyl-	416	C21H21F5O3	1010365-43-4	59
5			Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111723\
Data File : BP018256.D
Acq On : 18 Nov 2023 12:07
Operator : MA/JU
Sample : 05370-08
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCDQ4

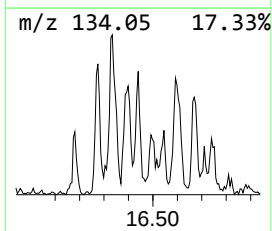
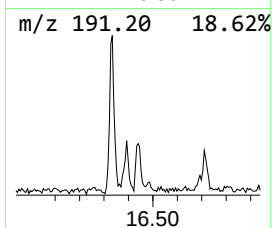
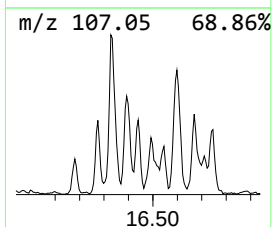
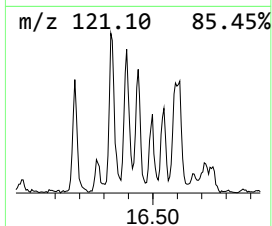
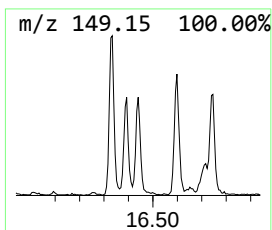
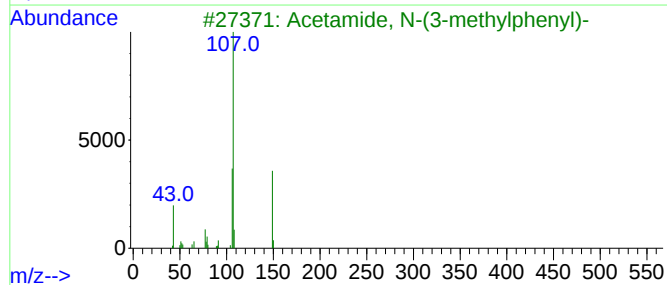
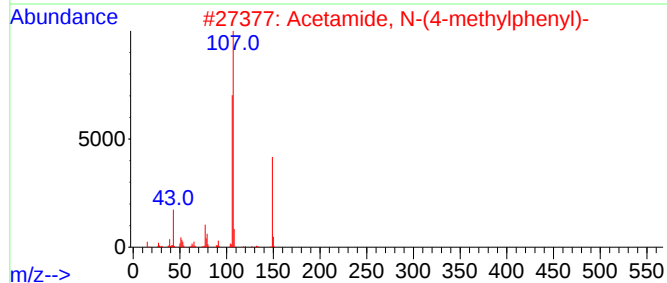
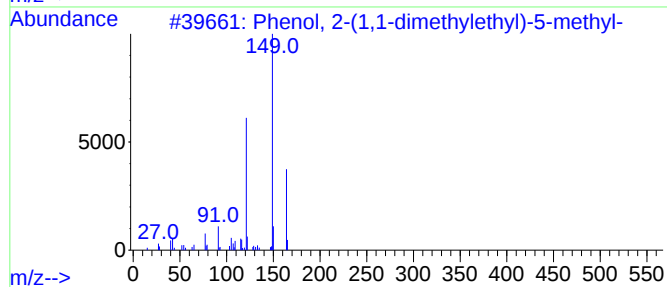
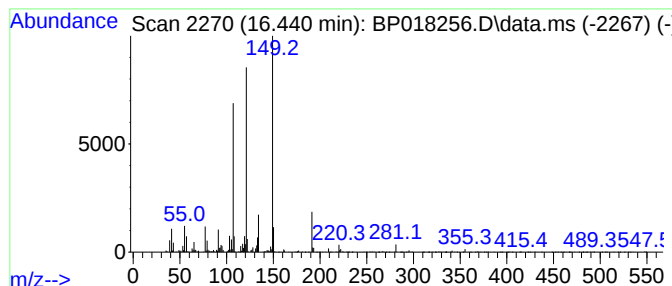
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 5 Phenol, 2-(1,1-dimethylethy... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.439	2.01 ng/ul	79405	Phenanthrene-d10	17.240

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2-(1,1-dimethylethyl)-5-...	164	C11H16O	000088-60-8	53
2			Acetamide, N-(4-methylphenyl)-	149	C9H11NO	000103-89-9	43
3			Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	43
4			Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	38
5			Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111723\
Data File : BP018256.D
Acq On : 18 Nov 2023 12:07
Operator : MA/JU
Sample : 05370-08
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCDQ4

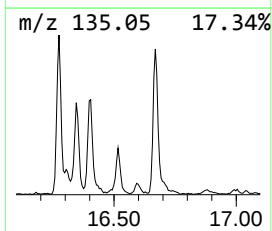
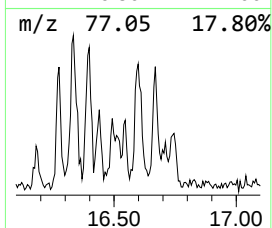
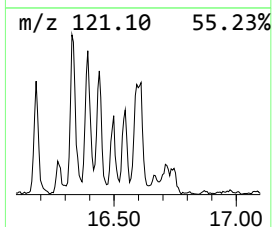
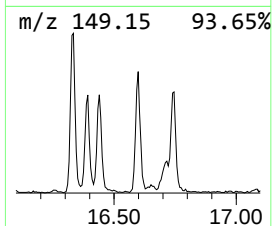
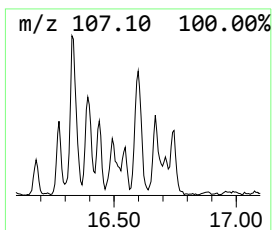
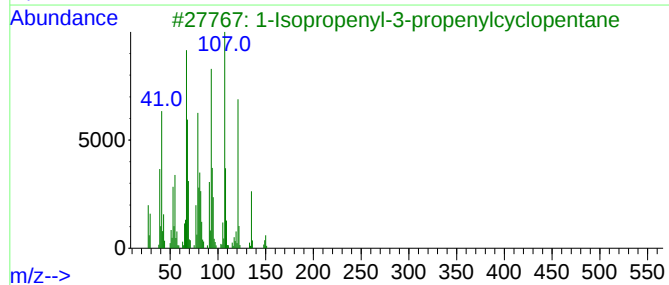
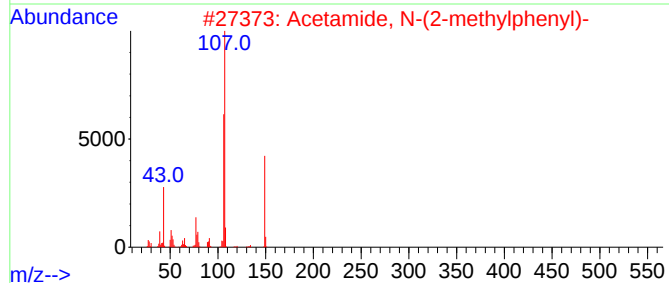
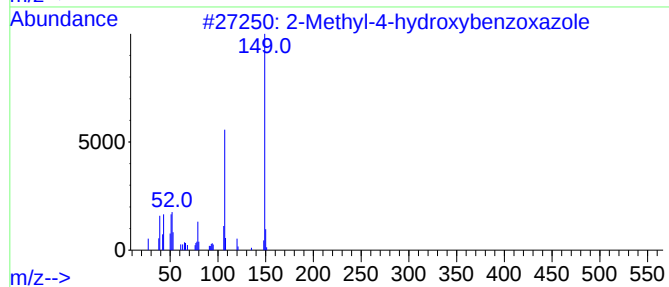
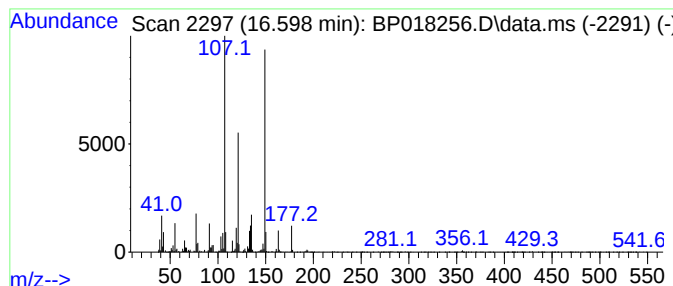
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 6 2-Methyl-4-hydroxybenzoxazole Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.598	3.89 ng/ul	153828	Phenanthrene-d10	17.240

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	53
2			Acetamide, N-(2-methylphenyl)-	149	C9H11NO	000120-66-1	46
3			1-Isopropenyl-3-propenylcyclopentane	150	C11H18	1000192-81-2	46
4			Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	43
5			Ethanol, 2-(3,3-dimethylbicyclo[...]	166	C11H18O	002226-05-3	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111723\
Data File : BP018256.D
Acq On : 18 Nov 2023 12:07
Operator : MA/JU
Sample : 05370-08
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCDQ4

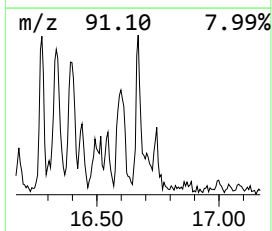
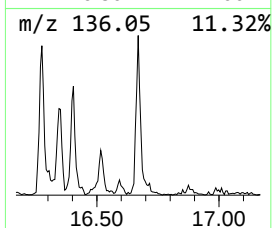
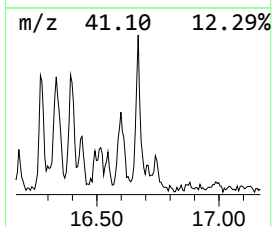
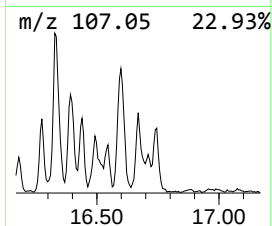
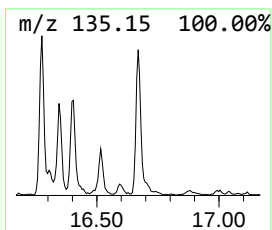
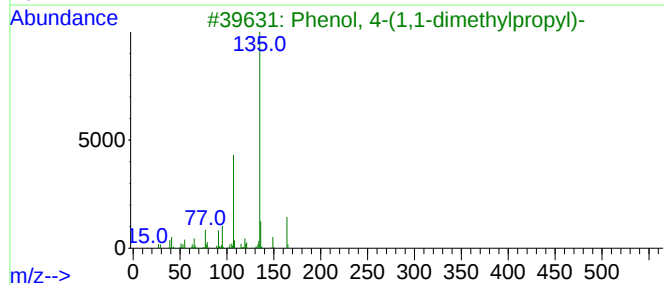
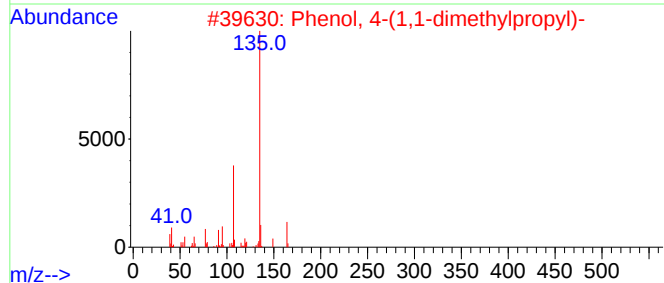
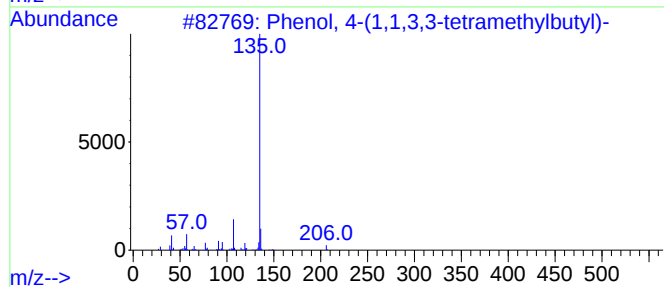
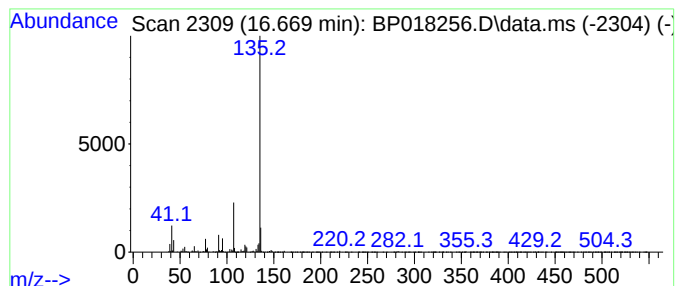
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 7 Phenol, 4-(1,1-dimethylprop... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.669	3.52 ng/ul	139084	Phenanthrene-d10	17.240

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	78
2			Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	78
3			Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	72
4			4-(1,1-Dimethylheptyl)phenol	220	C15H24O	1000384-80-3	72
5			Hexestrol	270	C18H22O2	000084-16-2	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111723\
Data File : BP018256.D
Acq On : 18 Nov 2023 12:07
Operator : MA/JU
Sample : 05370-08
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCDQ4

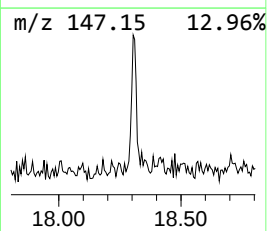
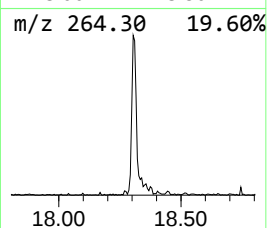
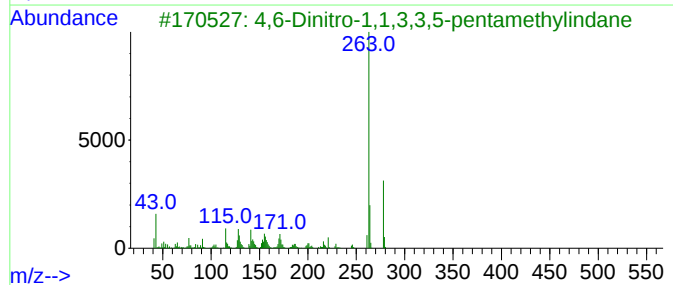
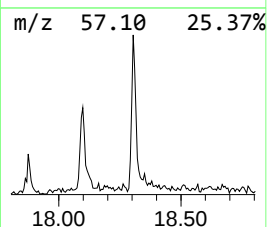
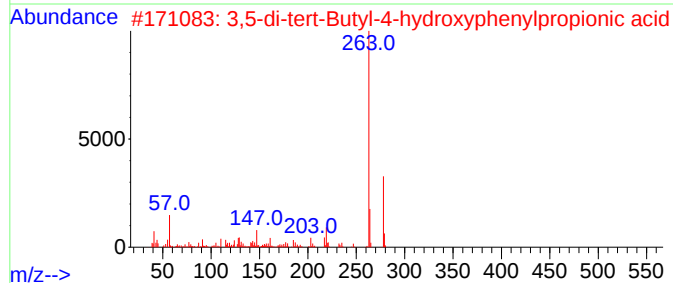
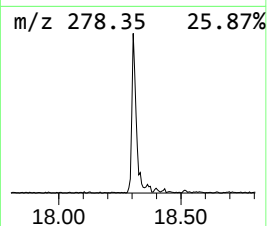
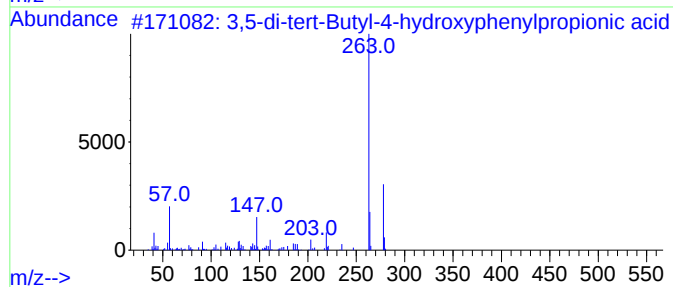
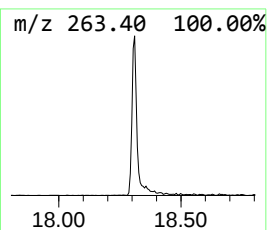
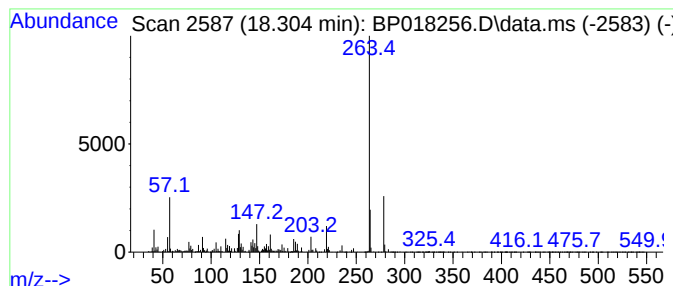
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 8 3,5-di-tert-Butyl-4-hydroxy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.304	2.72 ng/ul	107674	Phenanthrene-d10	17.240

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,5-di-tert-Butyl-4-hydroxypheny...	278	C17H26O3	020170-32-5	95
2			3,5-di-tert-Butyl-4-hydroxypheny...	278	C17H26O3	020170-32-5	93
3			4,6-Dinitro-1,1,3,3,5-pentamethy...	278	C14H18N2O4	000116-66-5	59
4			Cyanic acid, (1-methylethylidene...	278	C17H14N2O2	001156-51-0	59
5			7-Methyl-2-phenylquinoline-4-car...	263	C17H13NO2	181048-54-4	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111723\
Data File : BP018256.D
Acq On : 18 Nov 2023 12:07
Operator : MA/JU
Sample : 05370-08
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCDQ4

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

TIC Library : C:\DATABASE\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	13.299	6.5	ng/u1	187663	3	14.457	577736	20.0
Phenol, 4-(1,1,...	16.275	3.2	ng/u1	125132	4	17.240	791059	20.0
1-(Isocyanatome...	16.334	5.4	ng/u1	212213	4	17.240	791059	20.0
4-(7-Methylocty...	16.398	4.0	ng/u1	159718	4	17.240	791059	20.0
Phenol, 2-(1,1-...	16.439	2.0	ng/u1	79405	4	17.240	791059	20.0
2-Methyl-4-hydr...	16.598	3.9	ng/u1	153828	4	17.240	791059	20.0
Phenol, 4-(1,1-...	16.669	3.5	ng/u1	139084	4	17.240	791059	20.0
3,5-di-tert-But...	18.304	2.7	ng/u1	107674	4	17.240	791059	20.0