LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121121\
Data File : BP008373.D
Acq On : 11 Dec 2021 17:53
Operator : CG/JU
Sample : M4990-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
R1-COMP

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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\8270E-BP112521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008373.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.881	317	322	331	rBV	242081	332374	8.43%	1.646%
2	5.352	396	402	408	rBV	1222272	1808159	45.86%	8.955%
3	5.770	466	473	479	rVB	26545	40611	1.03%	0.201%
4	6.946	667	673	690	rBV	1081321	1924115	48.80%	9.529%
5	7.752	804	810	818	rBV	267655	419667	10.64%	2.078%
6	8.916	1001	1008	1028	rVB	735120	1248495	31.66%	6.183%
7	10.546	1278	1285	1294	rBV	318363	563300	14.29%	2.790%
8	13.022	1697	1706	1719	rBV	1724263	2549827	64.67%	12.628%
9	13.234	1736	1742	1746	rBV	30298	45035	1.14%	0.223%
10	14.404	1931	1941	1951	rBV	448954	707785	17.95%	3.505%
11	15.834	2179	2184	2190	rBV	89727	118745	3.01%	0.588%
12	15.910	2190	2197	2205	rBV	1271900	1843862	46.76%	9.131%
13	17.169	2405	2411	2416	rBV	580001	854964	21.68%	4.234%
14	17.292	2428	2432	2441	rVB4	68968	110282	2.80%	0.546%
15	17.463	2458	2461	2470	rBV2	30963	57853	1.47%	0.287%
16	17.828	2519	2523	2531	rVB2	76235	122137	3.10%	0.605%
17	18.075	2561	2565	2572	rBV	193851	287813	7.30%	1.425%
18	18.140	2572	2576	2579	rVB	60250	79467	2.02%	0.394%
19	19.198	2752	2756	2762	rBV	212313	349928	8.87%	1.733%
20	19.310	2772	2775	2783	rBV	101430	149208	3.78%	0.739%
21	19.745	2844	2849	2854	rVB	3407873	3943049	100.00%	19.527%
22	20.986	3057	3060	3070	rVB	318701	466850	11.84%	2.312%
23	21.186	3092	3094	3099	rVB	124409	138241	3.51%	0.685%
24	21.275	3105	3109	3114	rBV	779662	1042413	26.44%	5.162%
25	23.657	3508	3514	3522	rVB2	503607	988443	25.07%	4.895%

Sum of corrected areas: 20192623

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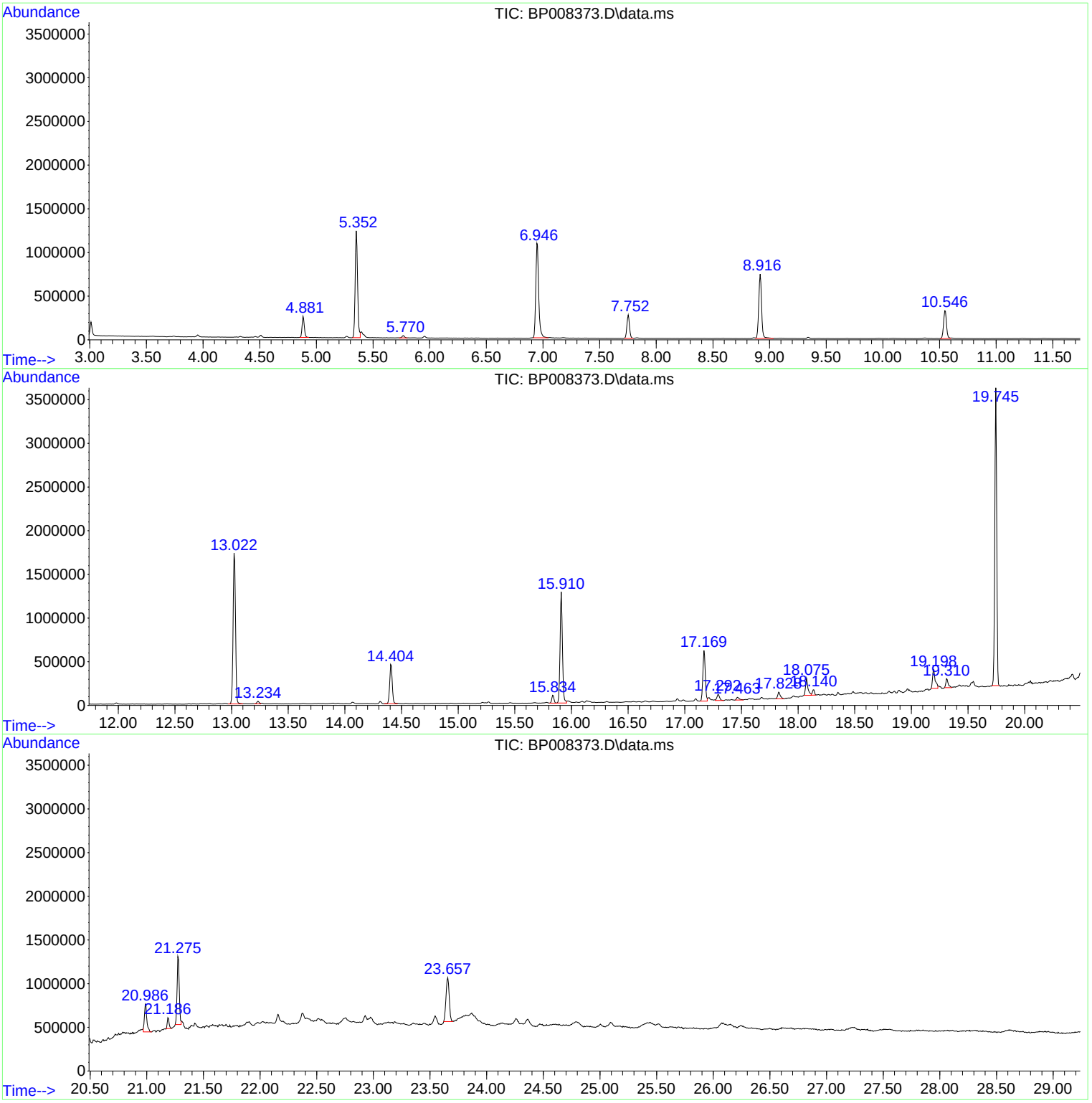
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BP008373.D
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Operator : CG/JU
Sample : M4990-15
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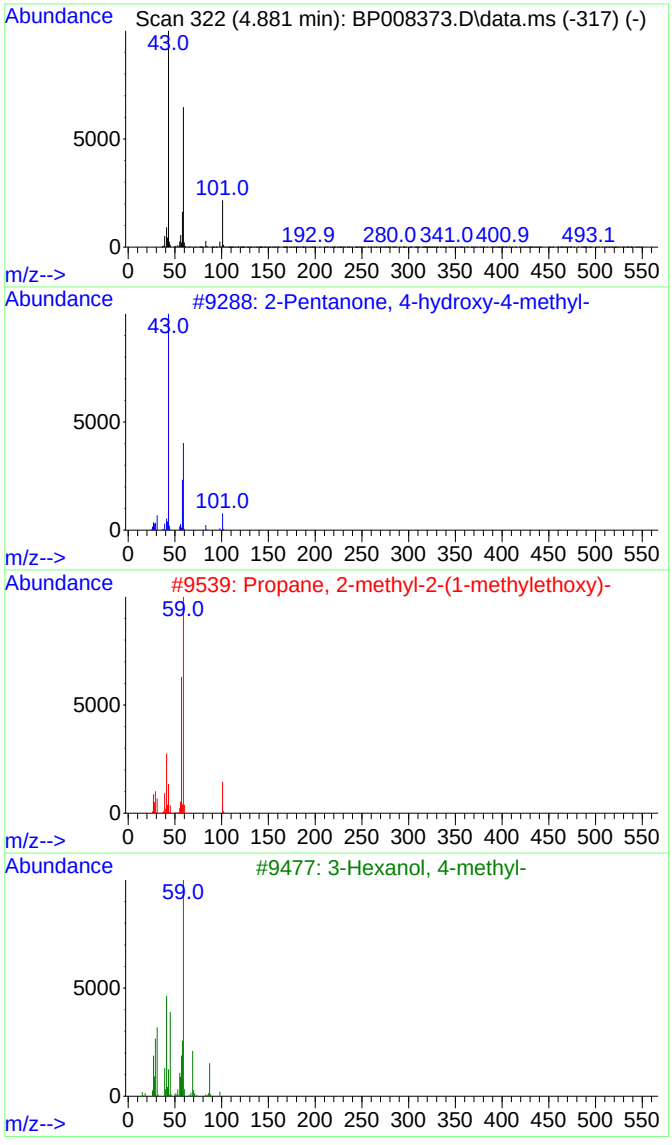
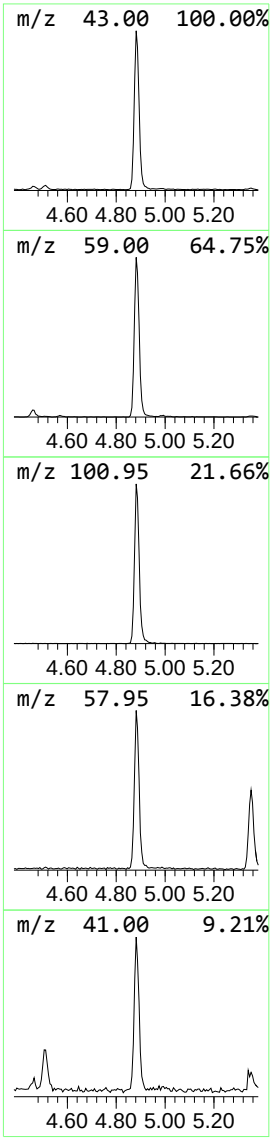
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.881	15.84 ng	332374	1,4-Dichlorobenzene-d4	7.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

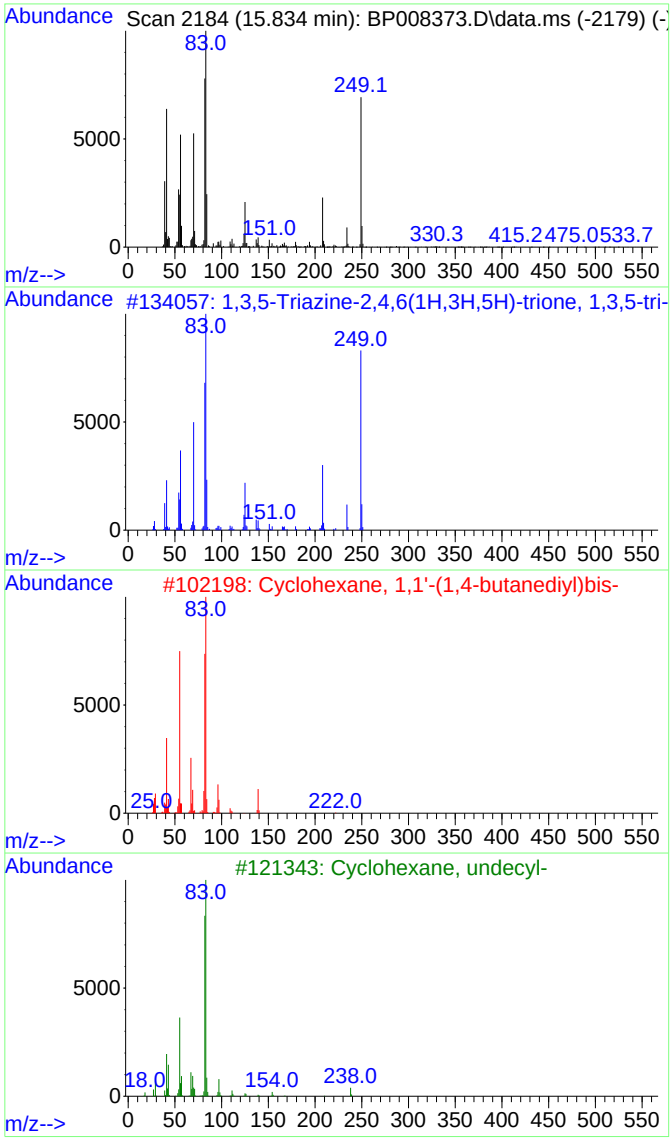
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

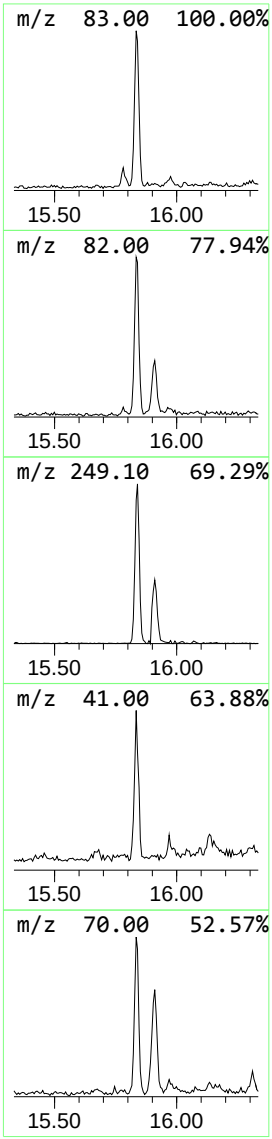
****

Peak Number 2 1,3,5-Triazine-2,4,6(1H,3H,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.834	2.78 ng	118745	Phenanthrene-d10	17.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine-2,4,6(1H,3H,5H)-t...	249	C12H15N3O3	001025-15-6	98
2	Cyclohexane, 1,1'-(1,4-butanediy...	222	C16H30	006165-44-2	35
3	Cyclohexane, undecyl-	238	C17H34	054105-66-7	32
4	Triallyl cyanurate	249	C12H15N3O3	000101-37-1	32
5	Cyclohexane, 1,1'-(1,3-propanedi...	208	C15H28	003178-24-3	16





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Operator : CG/JU
Sample : M4990-15
Misc :
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Instrument :
BNA_P
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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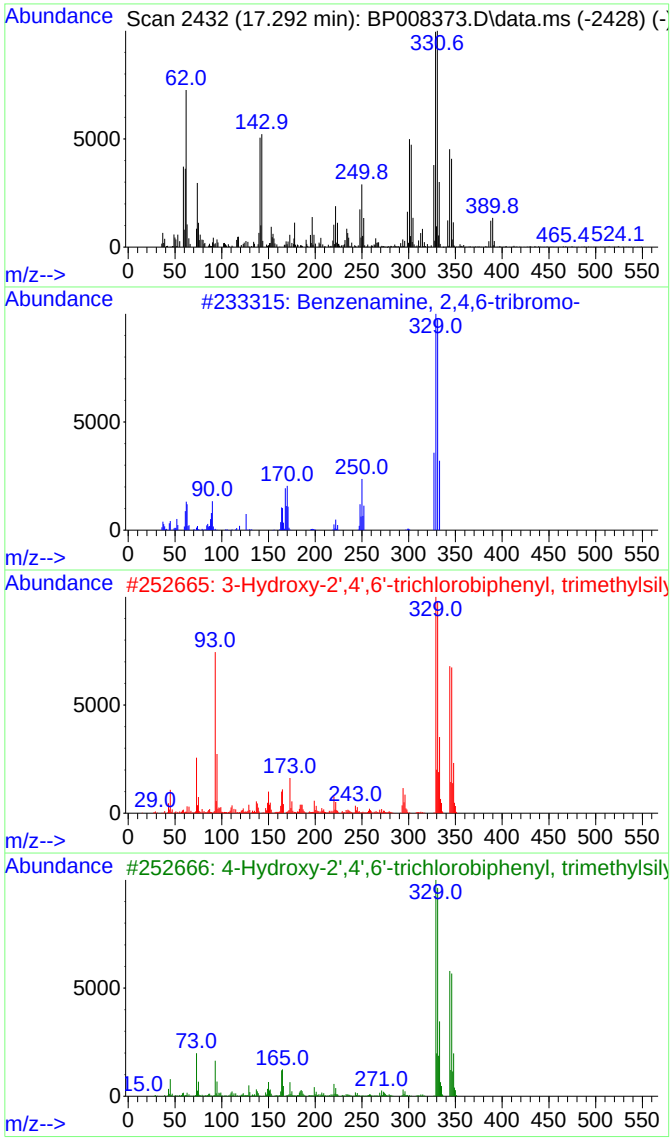
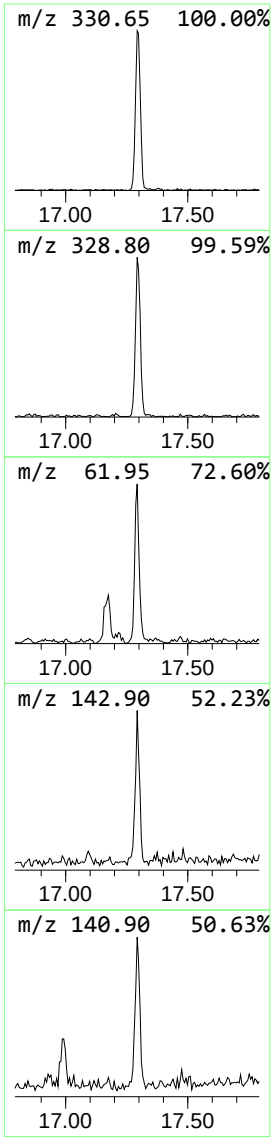
Peak Number 3 unknown17.293 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.293	2.58 ng	110282	Phenanthrene-d10	17.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 2,4,6-tribromo-	327	C6H4Br3N	000147-82-0	46
2	3-Hydroxy-2',4',6'-trichlorobiph...	344	C15H15Cl3OSi	1000447-69-8	41
3	4-Hydroxy-2',4',6'-trichlorobiph...	344	C15H15Cl3OSi	1000447-71-9	38
4	4-Hydroxy-2,2',5'-trichlorobiphe...	344	C15H15Cl3OSi	1000447-70-4	18
5	4-Hydroxy-2',4',6'-trichlorobiph...	386	C18H21Cl3OSi	1000447-71-7	18





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

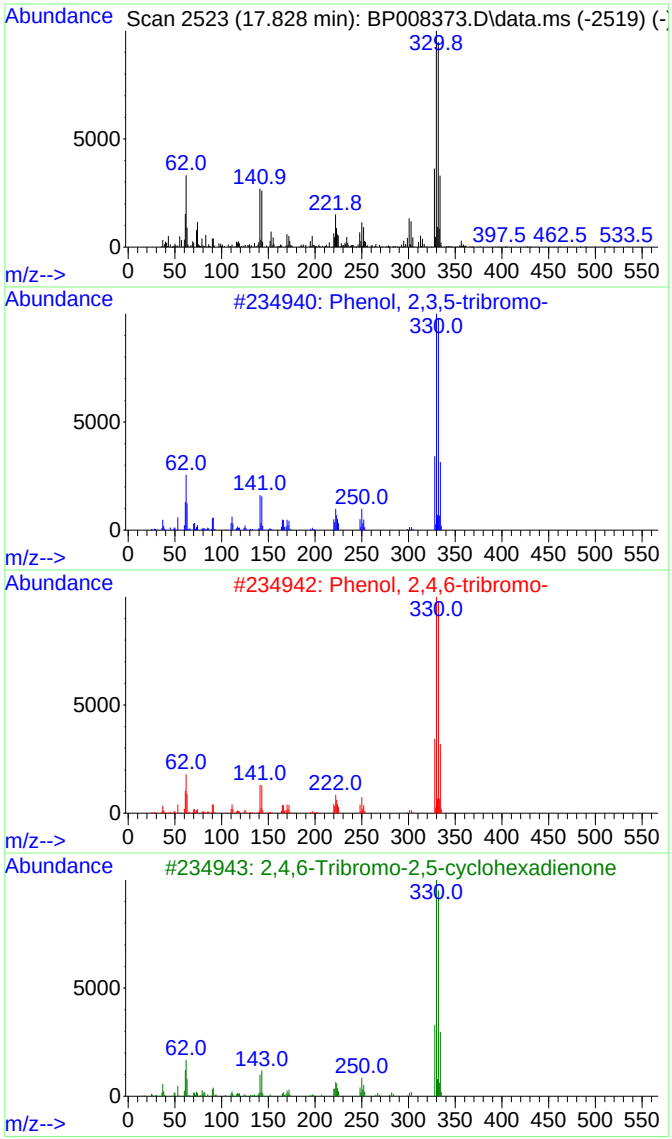
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

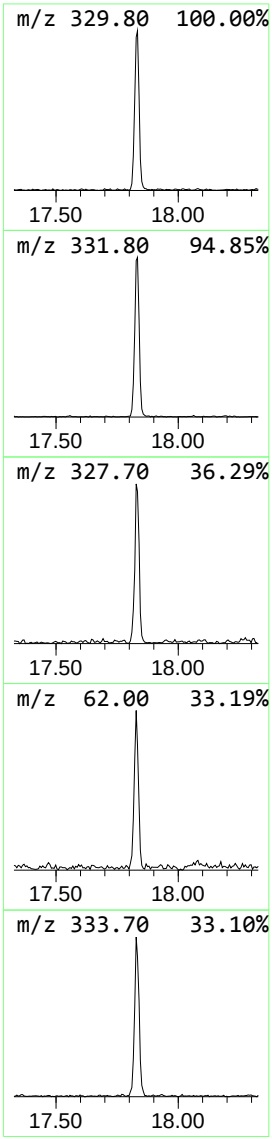
****

Peak Number 4 Phenol, 2,3,5-tribromo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.828	2.86 ng	122137	Phenanthrene-d10	17.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,3,5-tribromo-	328	C6H3Br3O	057383-81-0	99
2	Phenol, 2,4,6-tribromo-	328	C6H3Br3O	000118-79-6	98
3	2,4,6-Tribromo-2,5-cyclohexadienone	328	C6H3Br3O	020244-61-5	94
4	3,4,5-Tribromophenol	328	C6H3Br3O	116434-90-3	93
5	2,3,4-Tribromophenol	328	C6H3Br3O	138507-65-0	93





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Operator : CG/JU
Sample : M4990-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
R1-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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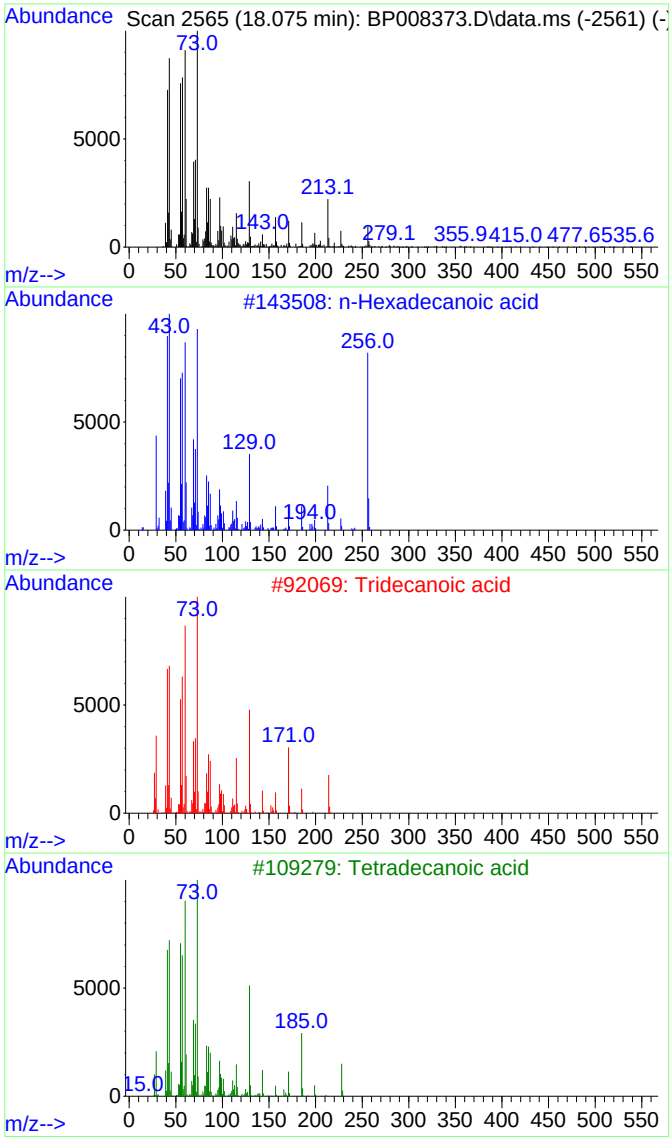
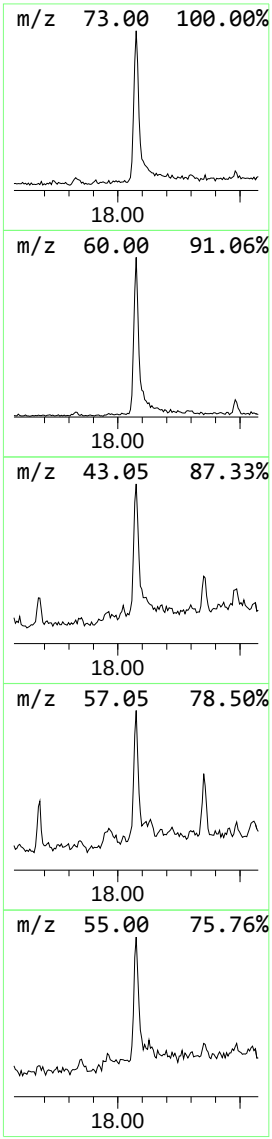
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.075	6.73 ng	287813	Phenanthrene-d10	17.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
4	Octadecanoic acid	284	C18H36O2	000057-11-4	87
5	Dodecanoic acid	200	C12H24O2	000143-07-7	87





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

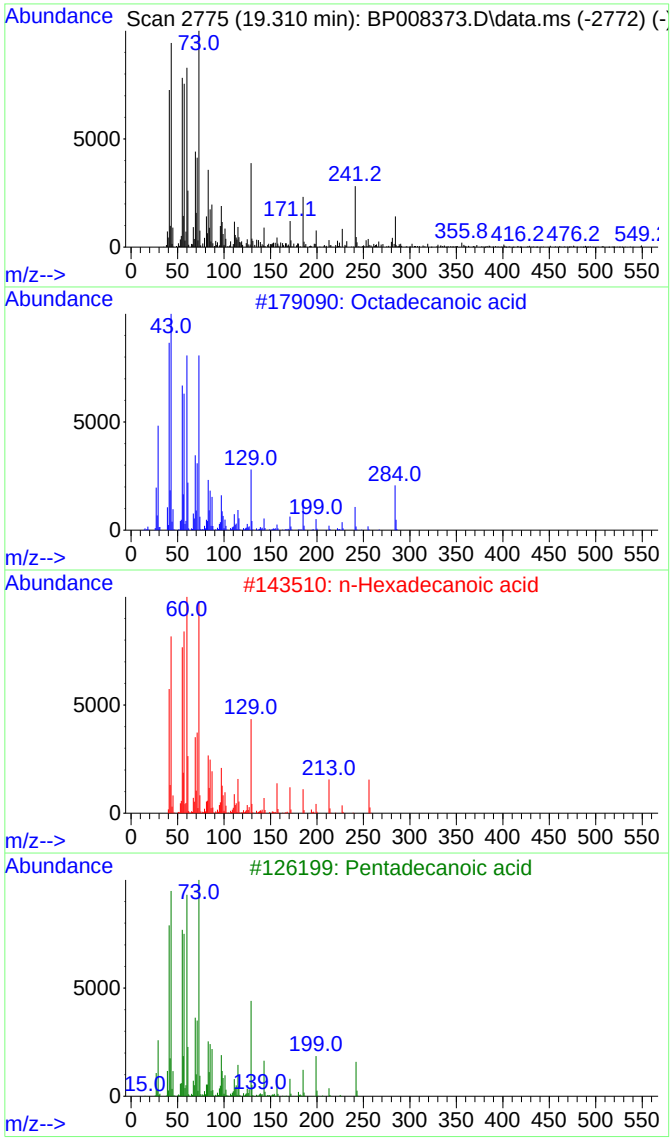
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

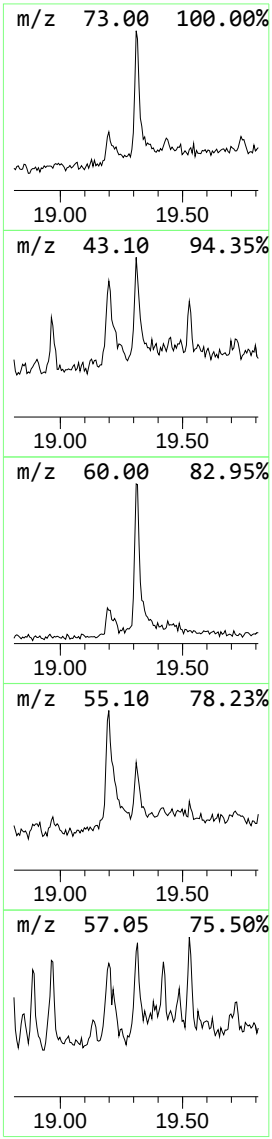
****

Peak Number 7 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.310	2.86 ng	149208	Chrysene-d12	21.275

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68





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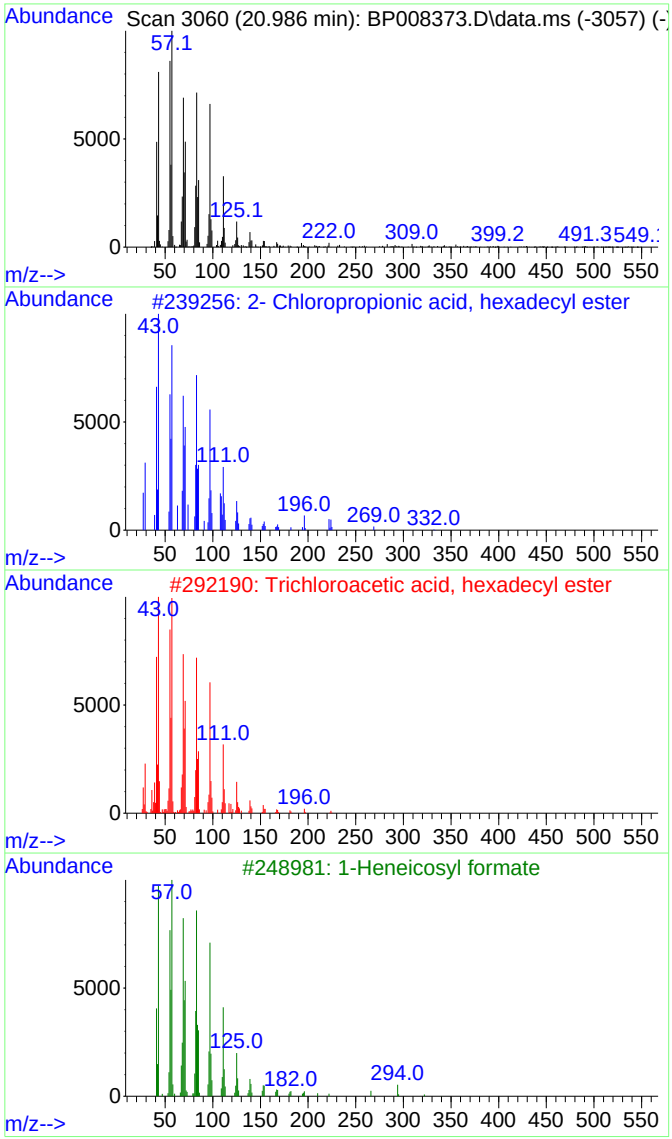
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

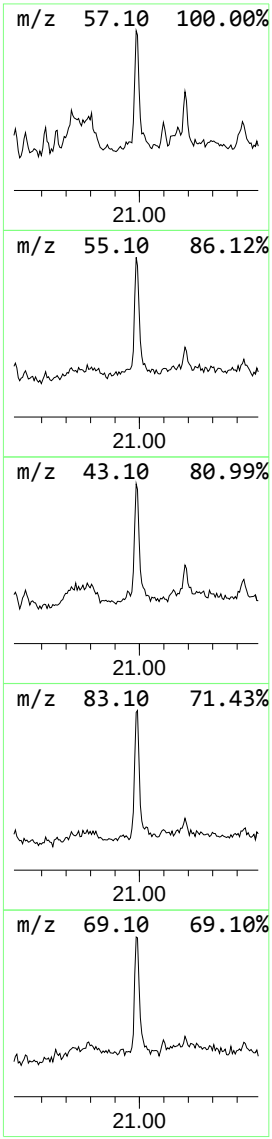
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 2- Chloropropionic acid, he... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.986	8.96 ng	466850	Chrysene-d12	21.275

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	95
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	93
4	1-Hexacosene	364	C26H52	018835-33-1	91
5	Cyclooctacosane	392	C28H56	000297-24-5	91





Tentatively Identified Compound (LSC) summary

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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-...	4.881	15.8	ng	332374	1	7.752	419667	20.0
1,3,5-Triazine-...	15.834	2.8	ng	118745	4	17.169	854964	20.0
unknown17.293	17.293	2.6	ng	110282	4	17.169	854964	20.0
Phenol, 2,3,5-t...	17.828	2.9	ng	122137	4	17.169	854964	20.0
n-Hexadecanoic ...	18.075	6.7	ng	287813	4	17.169	854964	20.0
Octadecanoic acid	19.310	2.9	ng	149208	5	21.275	1042410	20.0
2- Chloropropio...	20.986	9.0	ng	466850	5	21.275	1042410	20.0