

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121321\
 Data File : BP008383.D
 Acq On : 13 Dec 2021 18:59
 Operator : CG/JU
 Sample : M4990-13
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 R2-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: BP008383.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.952	160	164	168	rVB	23806	32397	1.09%	0.194%
2	4.505	255	258	264	rVB2	23624	32210	1.08%	0.193%
3	4.875	316	321	333	rBV	169661	250502	8.41%	1.501%
4	5.346	395	401	407	rBV	997301	1480590	49.70%	8.872%
5	5.763	466	472	480	rBV	22867	36683	1.23%	0.220%
6	6.940	661	672	694	rBV	833014	1509417	50.67%	9.044%
7	7.746	802	809	817	rBV	223843	352269	11.83%	2.111%
8	8.910	1001	1007	1022	rBV	555919	942484	31.64%	5.647%
9	10.546	1278	1285	1298	rBV	244130	447629	15.03%	2.682%
10	13.022	1698	1706	1721	rBV	1252586	1909058	64.09%	11.439%
11	14.304	1919	1924	1930	rBV2	20198	32301	1.08%	0.194%
12	14.404	1934	1941	1949	rBV	344629	542352	18.21%	3.250%
13	15.834	2178	2184	2189	rBV	70163	89668	3.01%	0.537%
14	15.904	2189	2196	2205	rBV	947491	1457837	48.94%	8.735%
15	17.169	2404	2411	2415	rVV	434332	652387	21.90%	3.909%
16	17.210	2415	2418	2425	rVV	85340	130678	4.39%	0.783%
17	17.292	2428	2432	2439	rVB2	40894	77121	2.59%	0.462%
18	17.828	2519	2523	2530	rVB2	33859	57636	1.93%	0.345%
19	18.069	2557	2564	2572	rBV2	233634	386049	12.96%	2.313%
20	18.133	2572	2575	2579	rVB	34360	43630	1.46%	0.261%
21	19.192	2750	2755	2763	rBV	173460	246343	8.27%	1.476%
22	19.310	2771	2775	2783	rVB	87130	125699	4.22%	0.753%
23	19.545	2808	2815	2824	rVB	126511	235706	7.91%	1.412%
24	19.739	2843	2848	2855	rVB	2509898	2978823	100.00%	17.849%
25	20.492	2973	2976	2978	rVB	40309	43259	1.45%	0.259%
26	20.986	3056	3060	3068	rVB3	343093	472814	15.87%	2.833%
27	21.186	3091	3094	3099	rVB	108520	118657	3.98%	0.711%
28	21.274	3103	3109	3113	rBV	764676	1070727	35.94%	6.416%
29	23.651	3508	3513	3521	rVB2	493181	934020	31.36%	5.597%

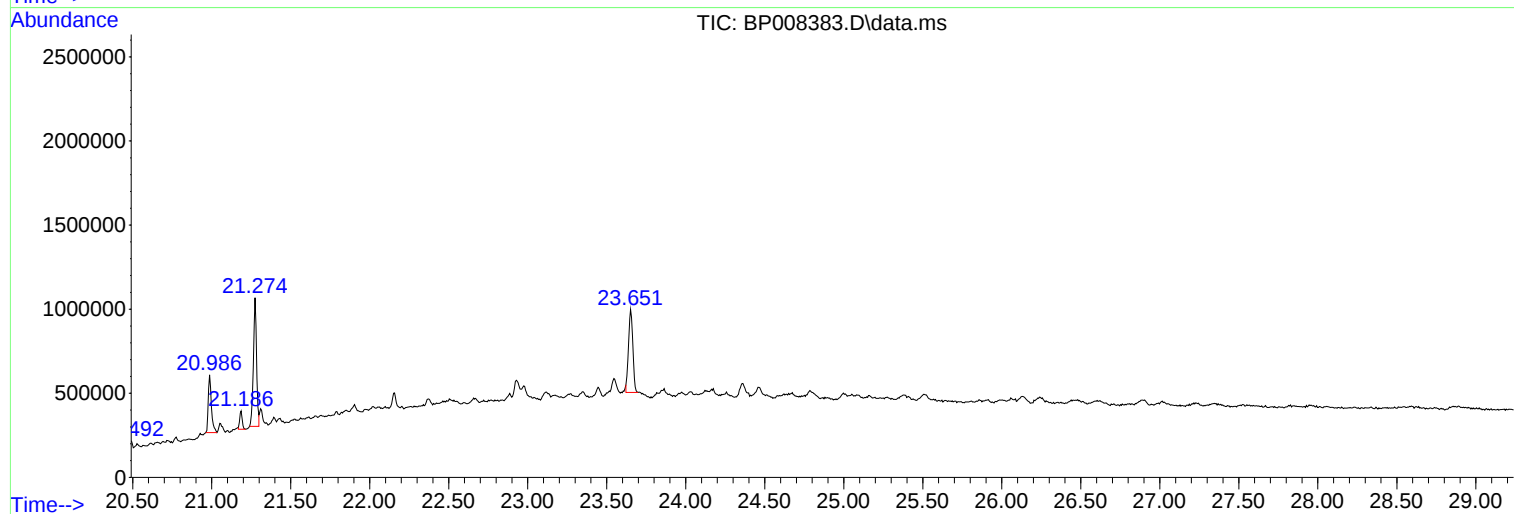
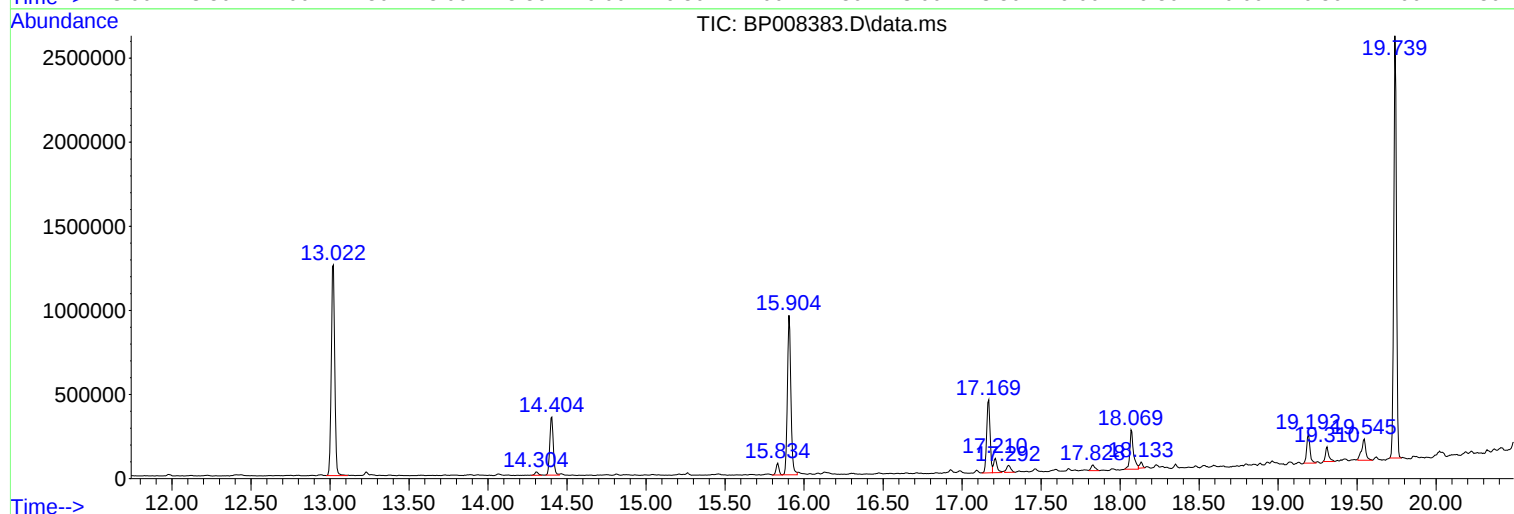
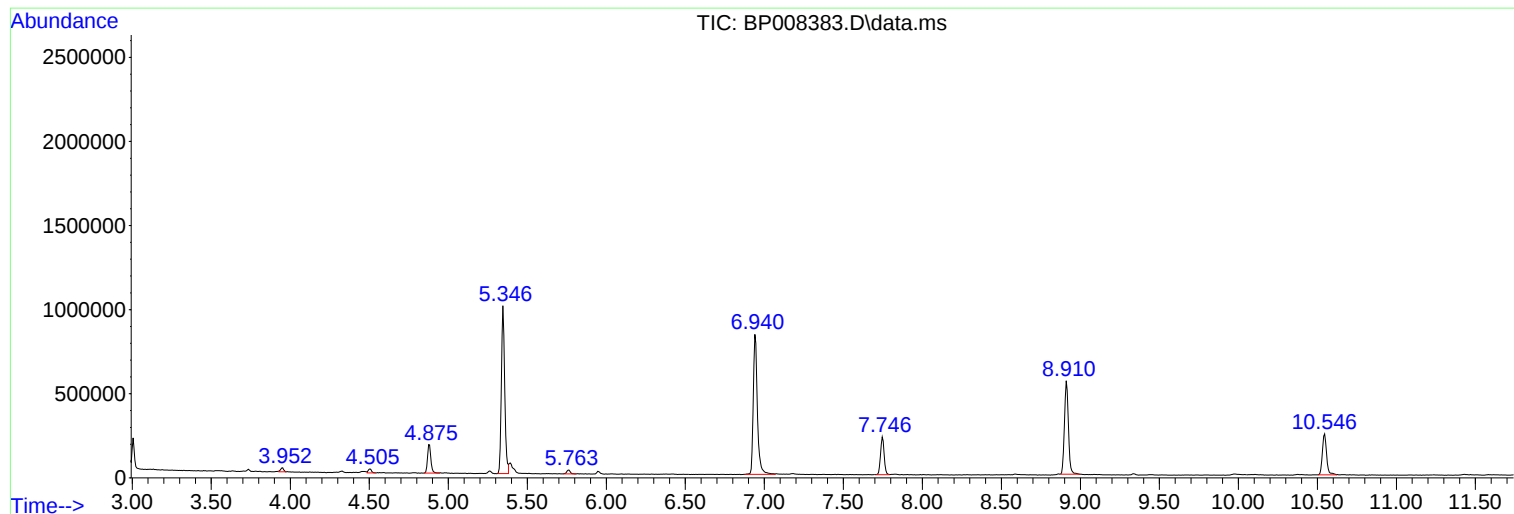
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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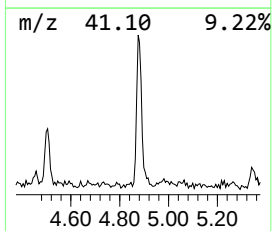
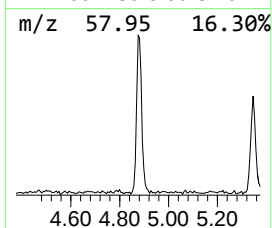
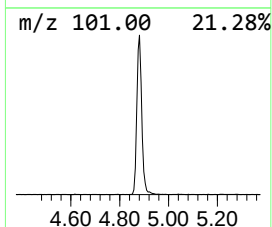
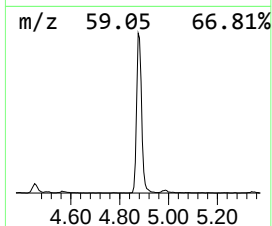
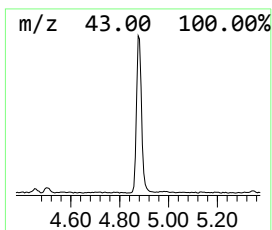
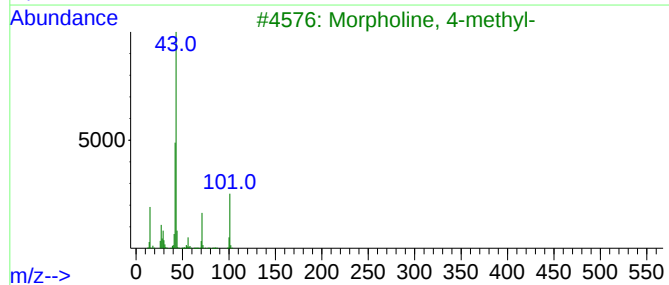
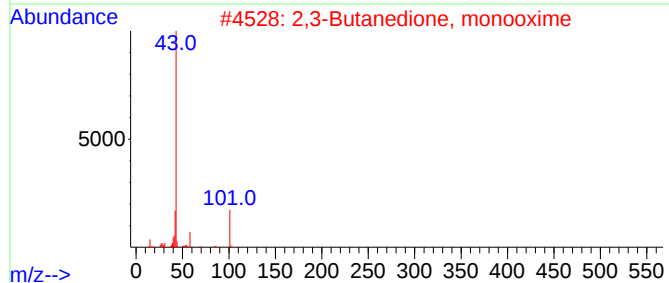
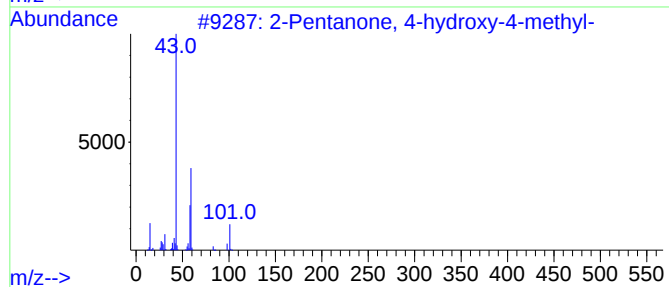
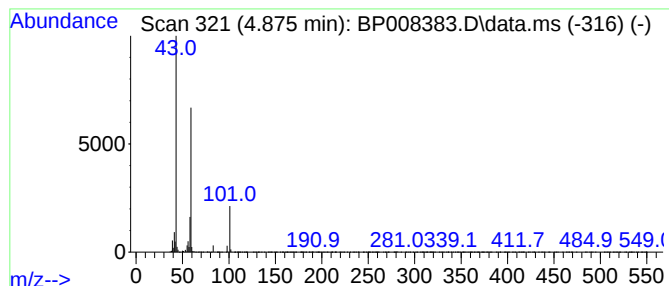
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.875	14.22 ng	250502	1,4-Dichlorobenzene-d4	7.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9		
5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9		



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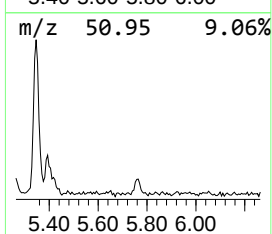
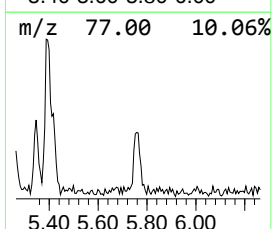
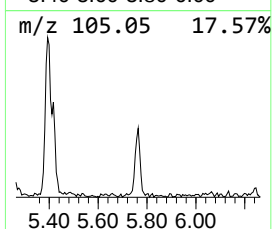
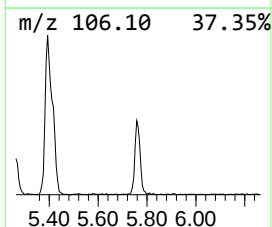
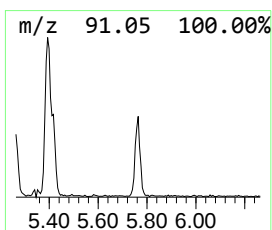
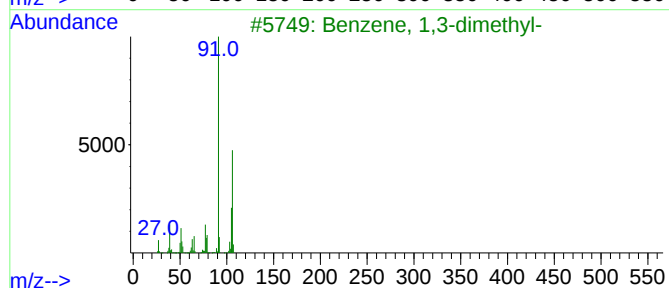
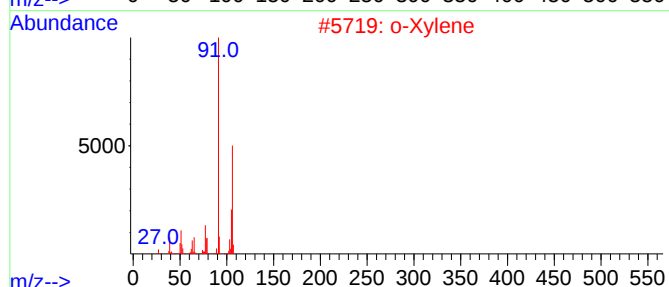
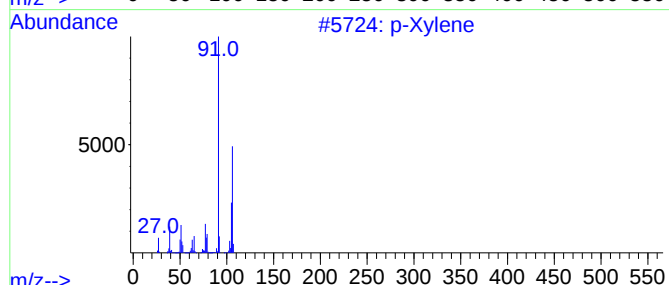
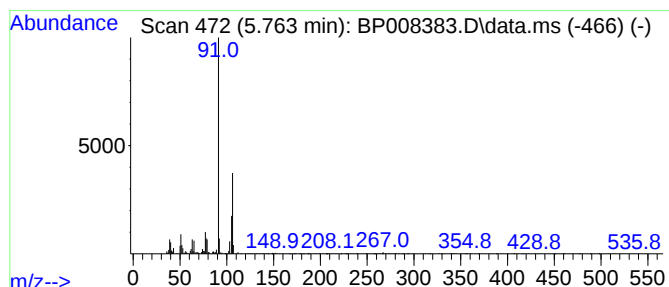
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 p-Xylene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.763	2.08 ng	36683	1,4-Dichlorobenzene-d4	7.746

Hit#	of 4	Tentative ID	MW	MolForm	CAS#	Qual
1		p-Xylene	106	C8H10	000106-42-3	95
2		o-Xylene	106	C8H10	000095-47-6	95
3		Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	95
4		Ethylbenzene	106	C8H10	000100-41-4	87



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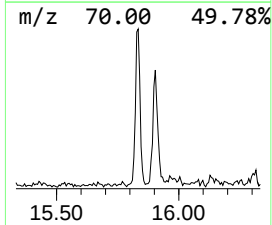
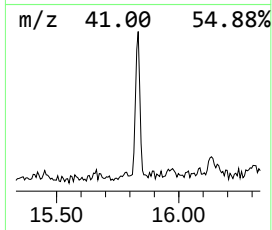
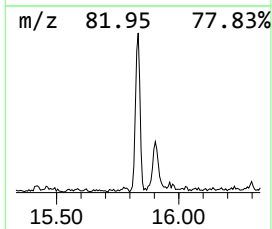
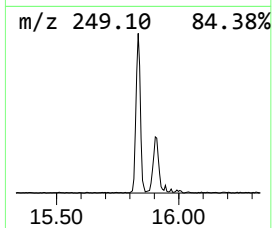
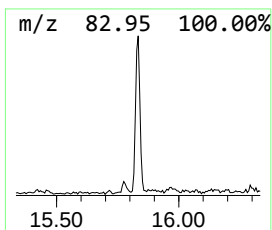
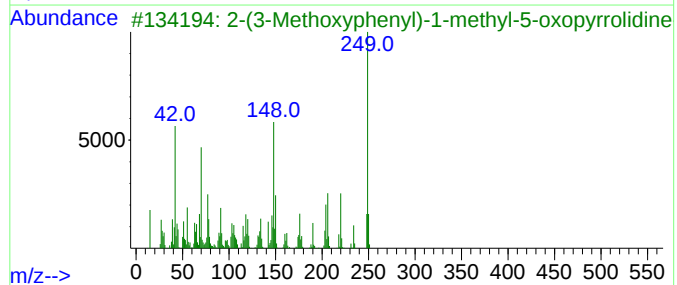
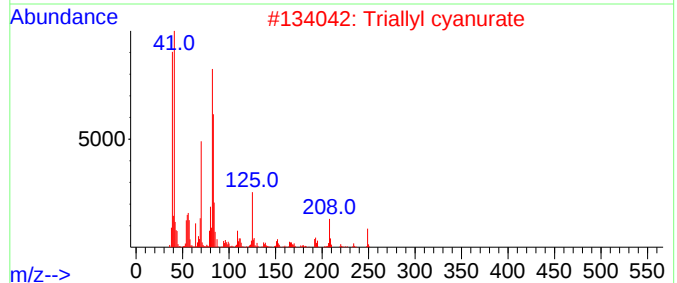
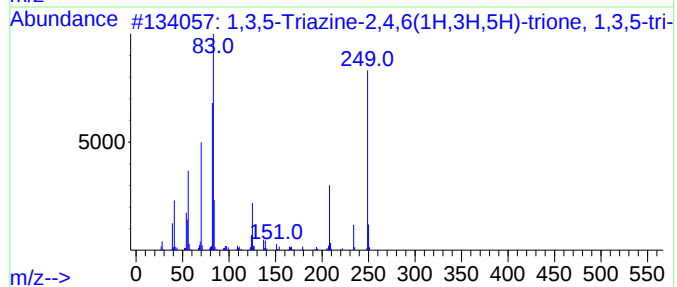
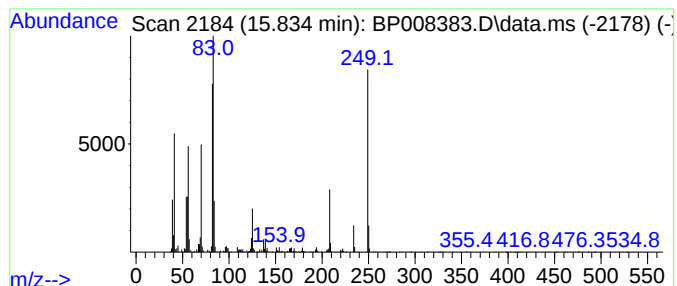
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.834	2.75 ng	89668	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	99
2		Triallyl cyanurate	249	C12H15N3O3	000101-37-1	32
3		2-(3-Methoxyphenyl)-1-methyl-5-o...	249	C13H15NO4	1000460-19-1	22
4		Cyclohexane, tetradecyl-	280	C20H40	001795-18-2	16
5		Heneicosylcyclohexane	378	C27H54	026718-82-1	14



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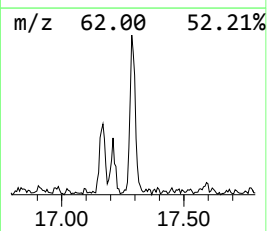
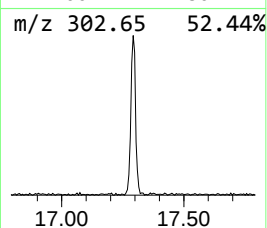
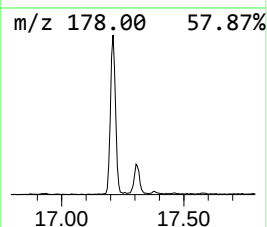
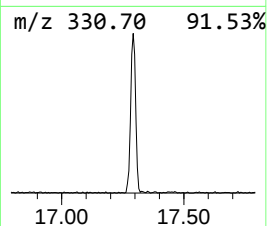
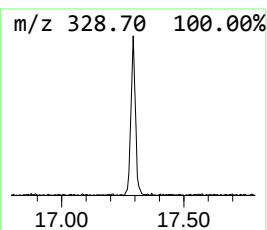
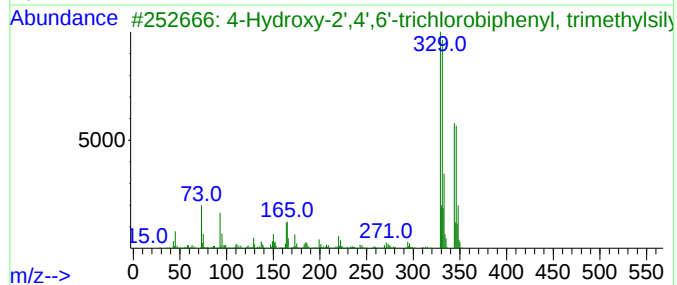
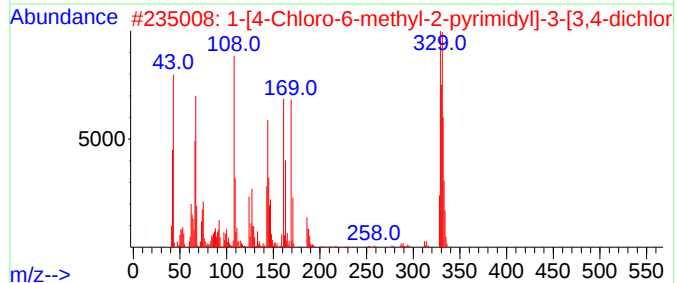
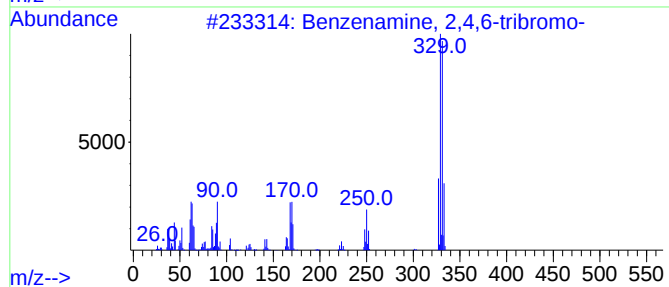
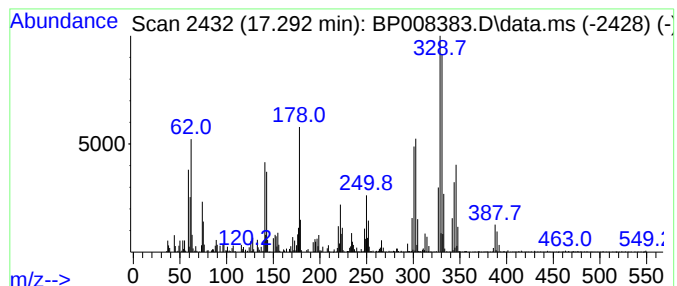
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Peak Number 4 unknown17.292 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.292	2.36 ng	77121	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			1-[4-Chloro-6-methyl-2-pyrimidyl...	329	C12H10Cl13N5	051387-79-2	30
3			4-Hydroxy-2',4',6'-trichlorobiph...	344	C15H15Cl3OSi	1000447-71-9	16
4			Cyclobutane, 1,2-dichloro-	124	C4H6Cl2	017437-39-7	14
5			4-Hydroxy-2',4',6'-trichlorobiph...	386	C18H21Cl3OSi	1000447-71-7	12



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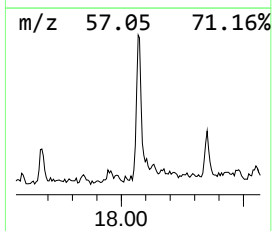
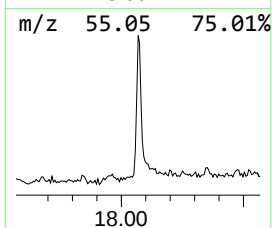
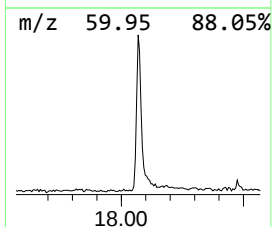
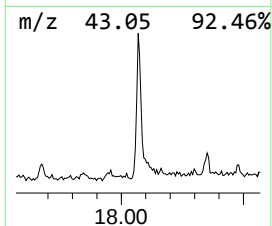
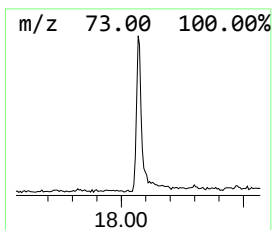
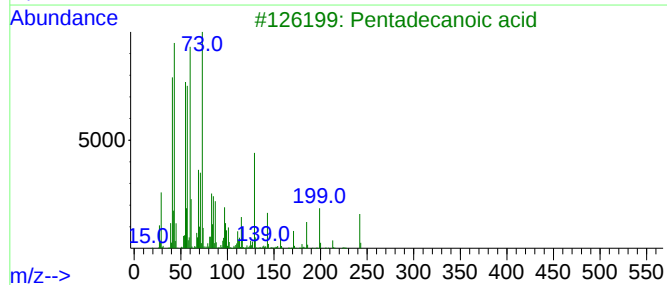
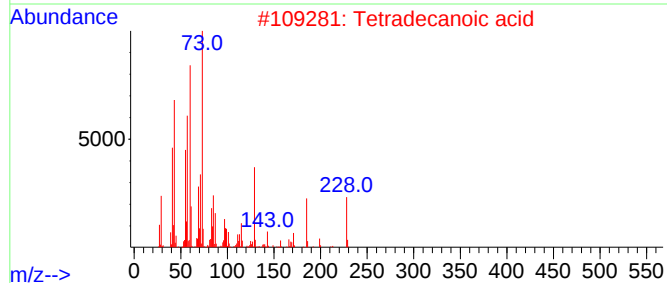
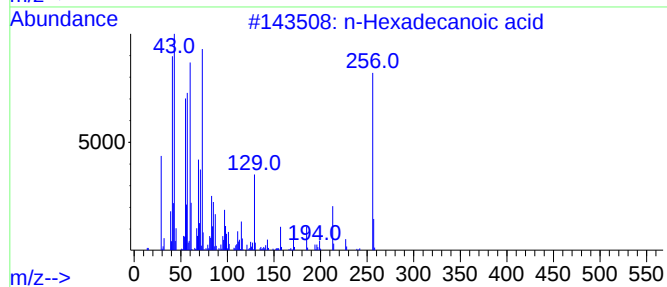
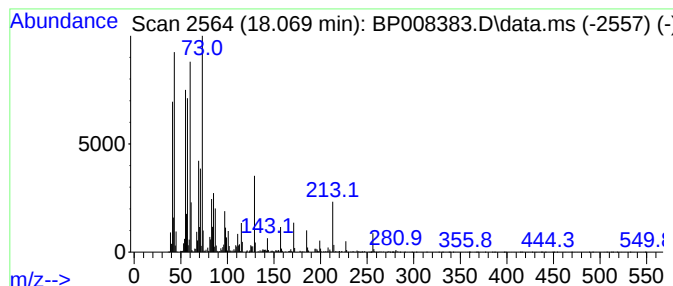
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.069	11.84 ng	386049	Phenanthrene-d10		17.169	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid		228	C14H28O2	000544-63-8	94
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	87
4	Tridecanoic acid		214	C13H26O2	000638-53-9	87
5	Dodecanoic acid		200	C12H24O2	000143-07-7	72



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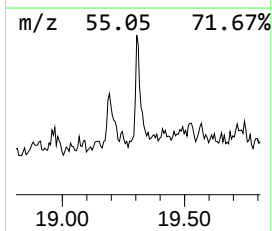
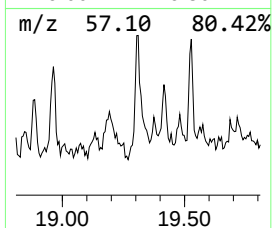
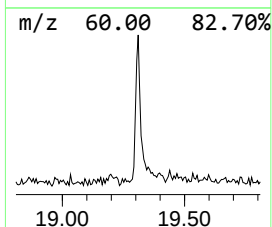
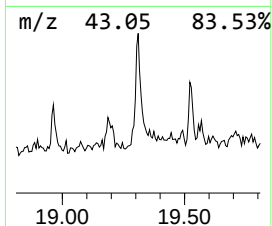
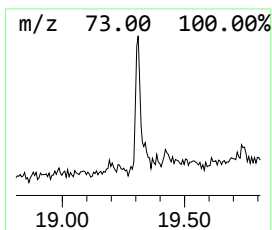
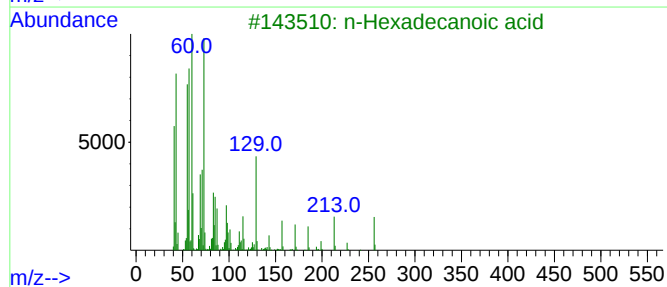
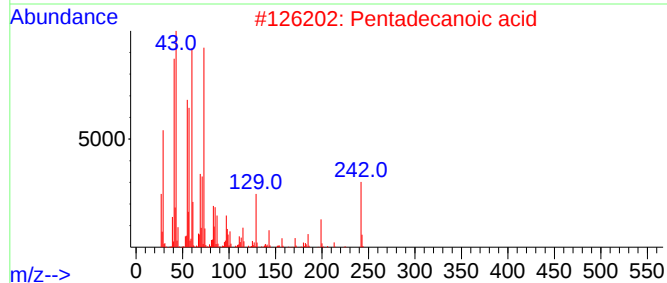
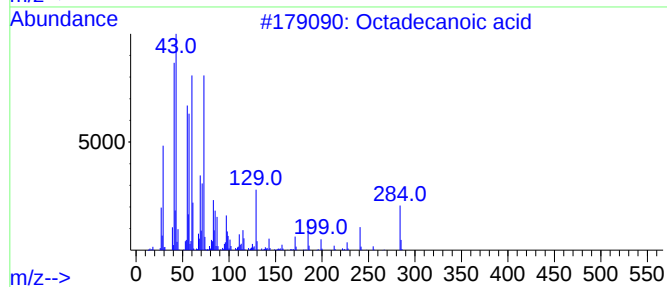
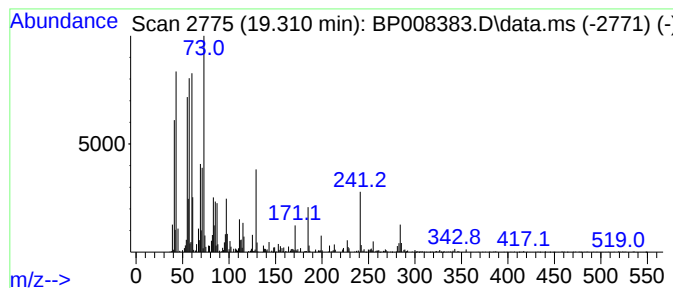
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.310	2.35 ng	125699	Chrysene-d12	21.274

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	95
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121321\
Data File : BP008383.D
Acq On : 13 Dec 2021 18:59
Operator : CG/JU
Sample : M4990-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
R2-COMP

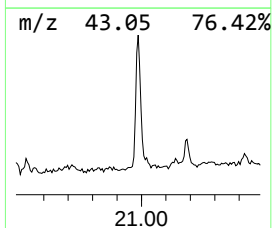
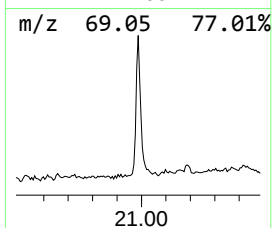
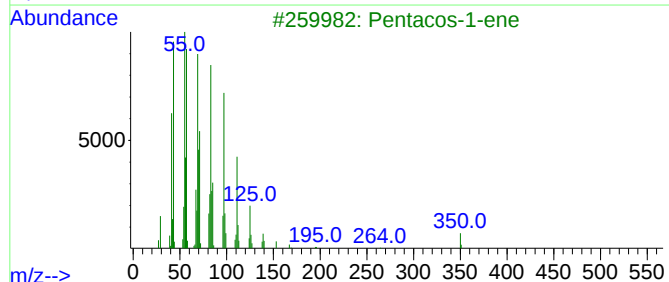
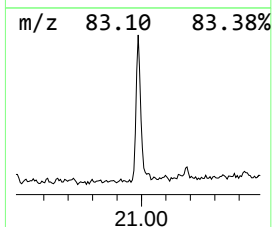
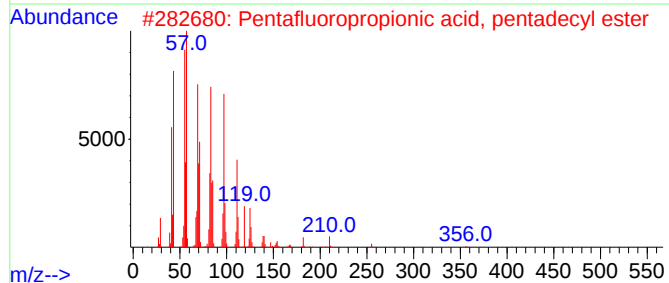
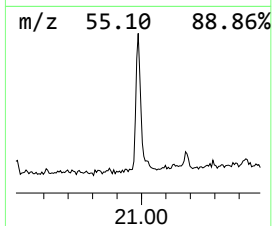
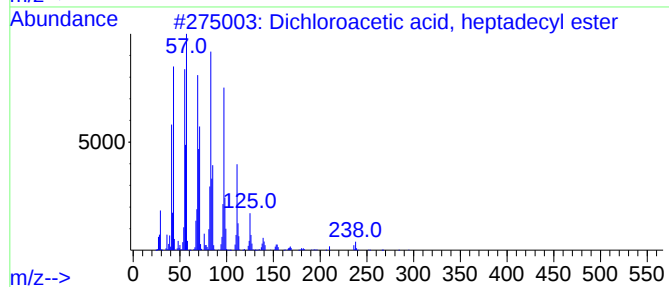
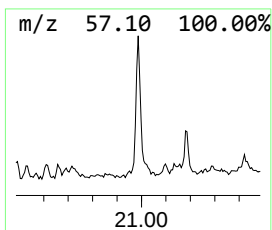
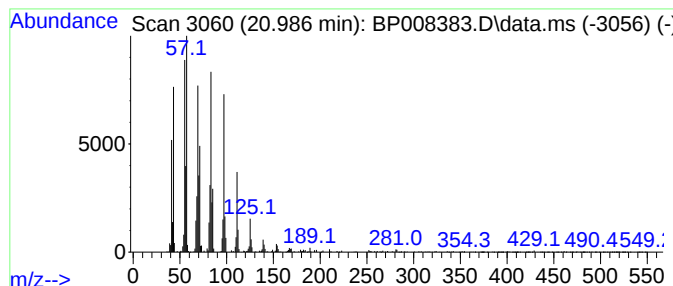
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Dichloroacetic acid, heptad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.986	8.83 ng	472814	Chrysene-d12	21.274

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3			Pentacos-1-ene	350	C25H50	016980-85-1	94
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121321\
Data File : BP008383.D
Acq On : 13 Dec 2021 18:59
Operator : CG/JU
Sample : M4990-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
R2-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
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.875	14.2	ng	250502	1	7.746	352269	20.0
p-Xylene	5.763	2.1	ng	36683	1	7.746	352269	20.0
1,3,5-Triazine-...	15.834	2.8	ng	89668	4	17.169	652387	20.0
unknown17.292	17.292	2.4	ng	77121	4	17.169	652387	20.0
n-Hexadecanoic ...	18.069	11.8	ng	386049	4	17.169	652387	20.0
Octadecanoic acid	19.310	2.4	ng	125699	5	21.274	1070730	20.0
Dichloroacetic ...	20.986	8.8	ng	472814	5	21.274	1070730	20.0