

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111222\
 Data File : BG055591.D
 Acq On : 12 Nov 2022 15:53
 Operator : CG/JU
 Sample : N5431-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20221176-COMP-11-MODIFIED-ELUTRIATE

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_G\Methods\8270-BG110922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055591.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.323	3	6	28	rVB	547969	845567	32.51%	5.231%
2	4.704	236	241	247	rBV	18912	27990	1.08%	0.173%
3	5.321	341	346	353	rBV	52524	77526	2.98%	0.480%
4	5.791	420	426	438	rVB	294355	471470	18.13%	2.917%
5	7.401	693	700	709	rBV	229003	391582	15.06%	2.423%
6	8.270	839	848	854	rBV	276556	478692	18.41%	2.961%
7	9.440	1039	1047	1056	rBV	340142	607803	23.37%	3.760%
8	11.097	1321	1329	1336	rBV	383633	692792	26.64%	4.286%
9	13.511	1732	1740	1747	rBV	944311	1492134	57.38%	9.231%
10	14.886	1965	1974	1984	rVB	684522	1062249	40.85%	6.572%
11	16.367	2219	2226	2241	rBV	909927	1416028	54.45%	8.760%
12	17.630	2432	2441	2447	rBV	921739	1419178	54.57%	8.780%
13	18.271	2545	2550	2556	rVB	34430	43595	1.68%	0.270%
14	18.488	2581	2587	2598	rBV	265501	408823	15.72%	2.529%
15	19.428	2743	2747	2751	rVB3	29545	33462	1.29%	0.207%
16	19.628	2774	2781	2792	rBV10	18089	52366	2.01%	0.324%
17	19.745	2796	2801	2809	rBV	89858	142716	5.49%	0.883%
18	20.215	2875	2881	2888	rVB	2056115	2600628	100.00%	16.089%
19	21.531	3100	3105	3120	rBV	177860	385707	14.83%	2.386%
20	21.925	3165	3172	3183	rVB2	947717	1621954	62.37%	10.034%
21	23.705	3470	3475	3482	rVB	62539	124091	4.77%	0.768%
22	25.356	3744	3756	3772	rVB2	548061	1767635	67.97%	10.936%

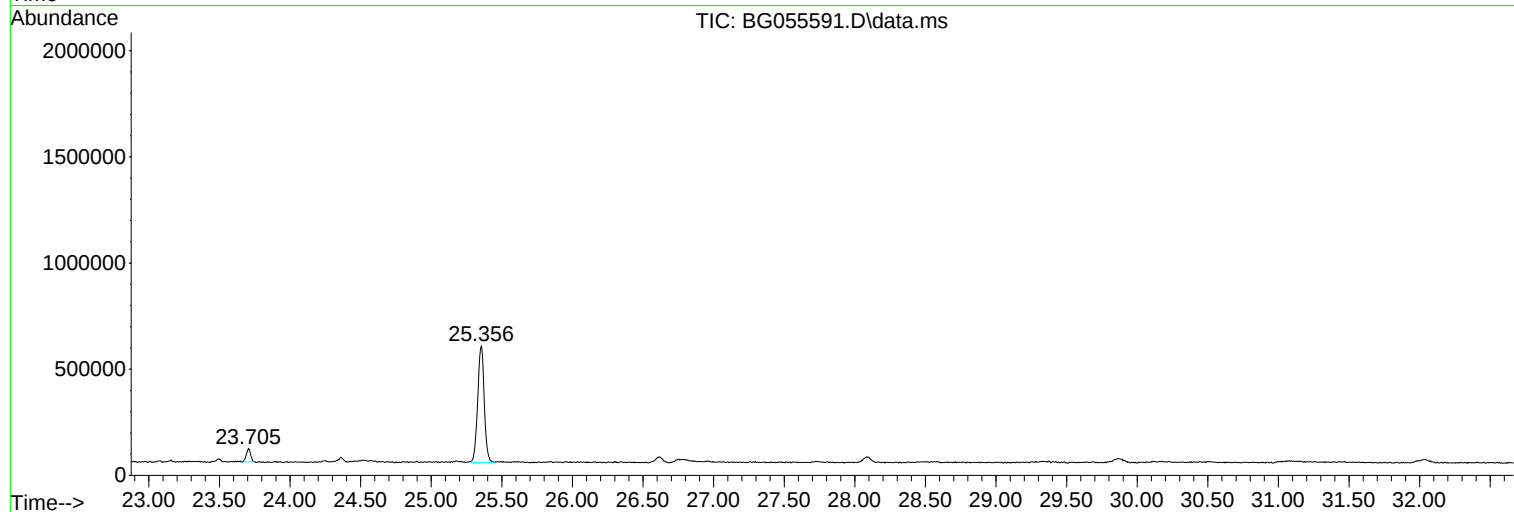
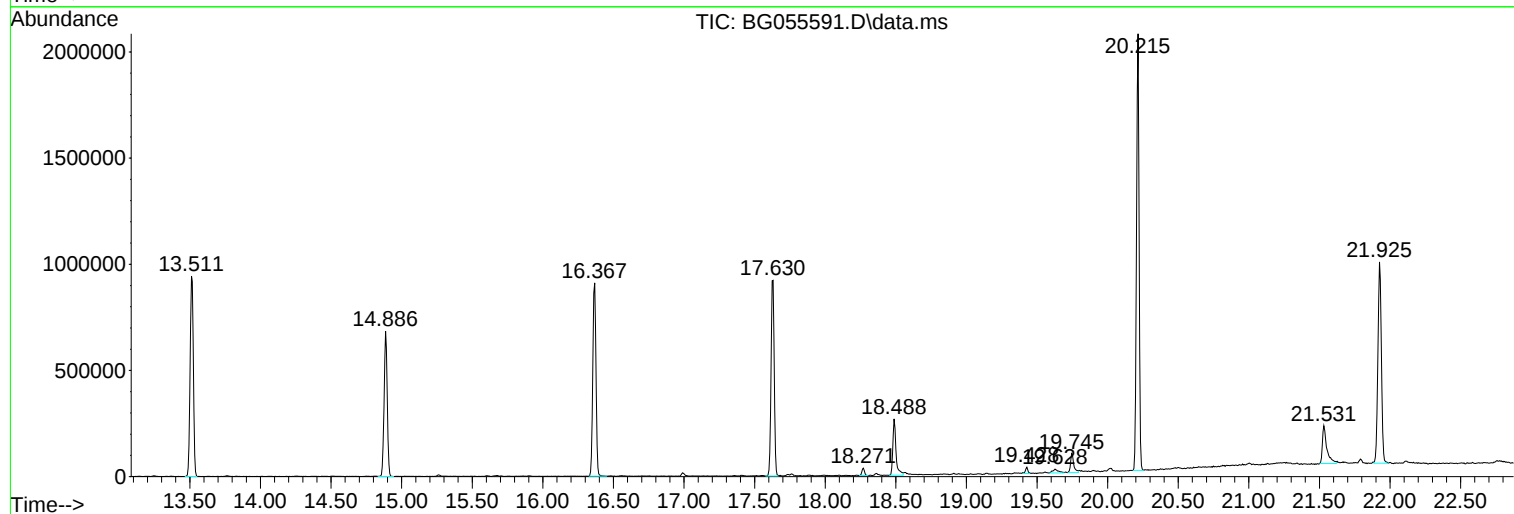
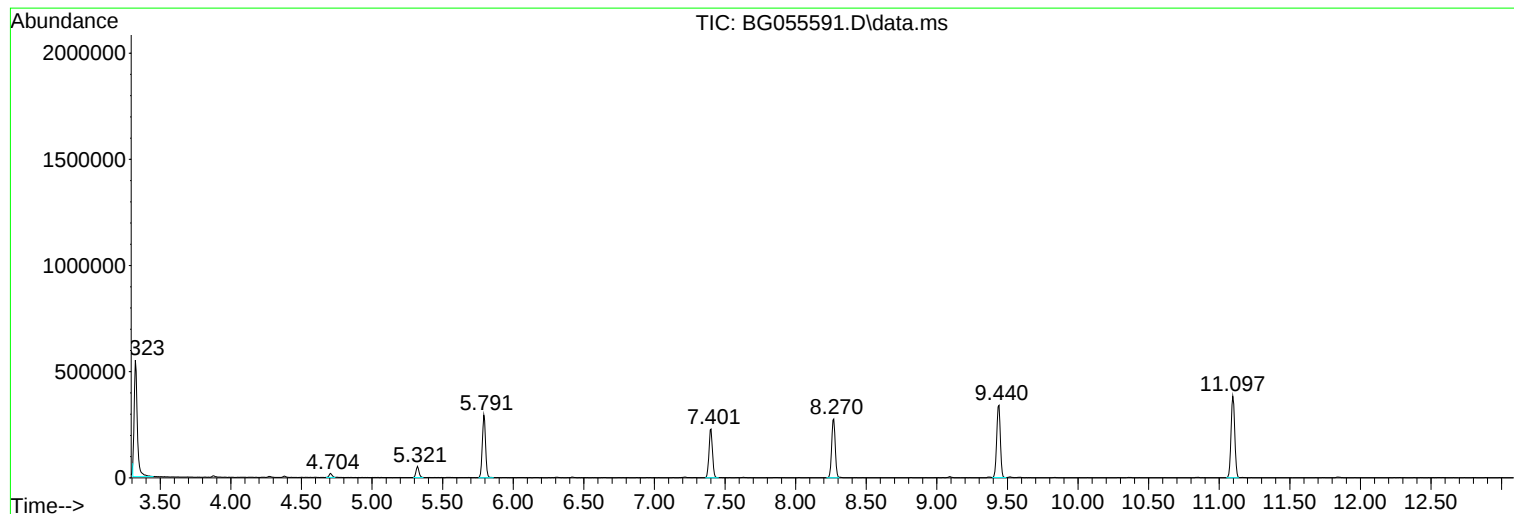
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ClientSampleId :
20221176-COMP-11-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.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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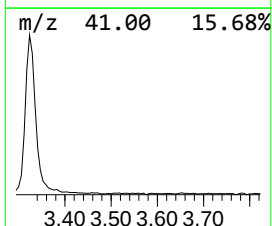
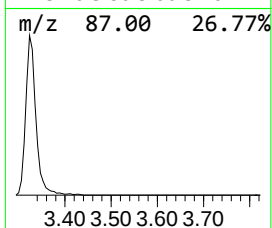
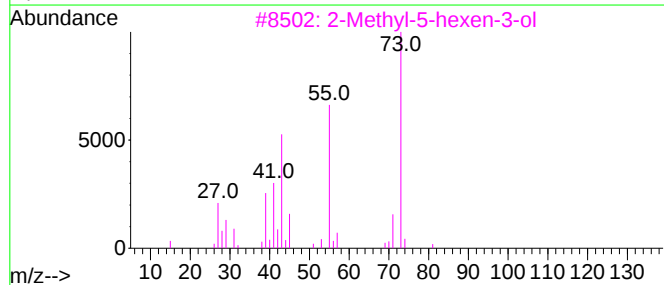
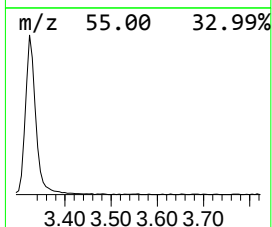
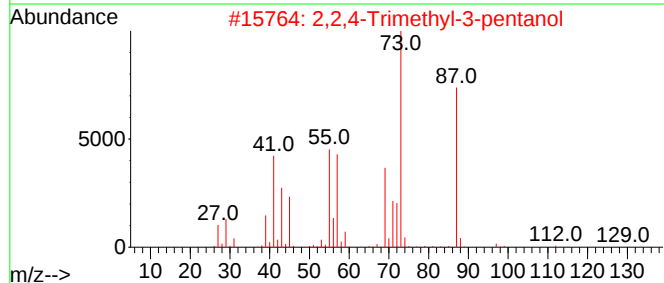
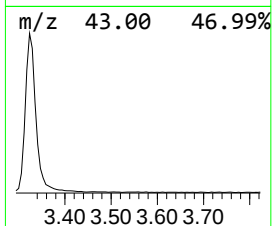
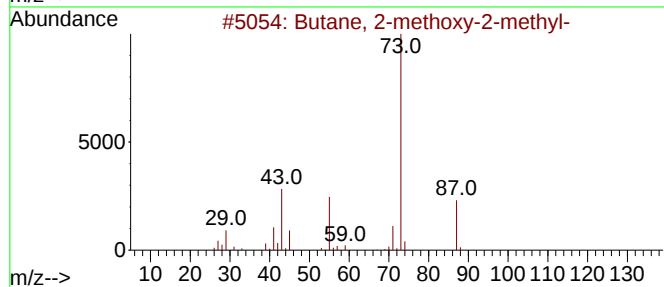
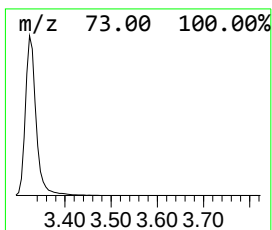
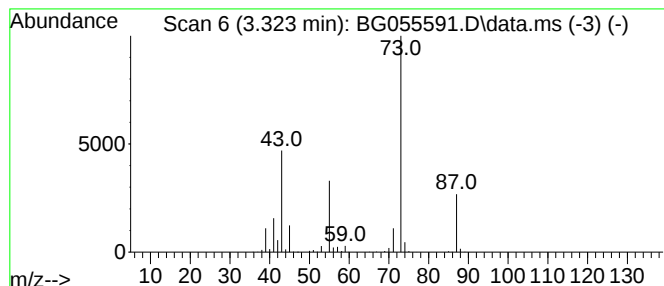
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.323	35.33 ng	845567	1,4-Dichlorobenzene-d4	8.270

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	28
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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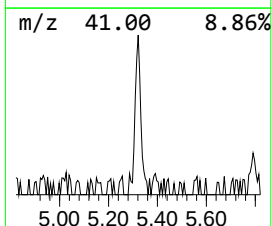
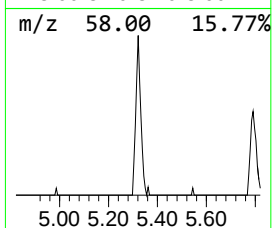
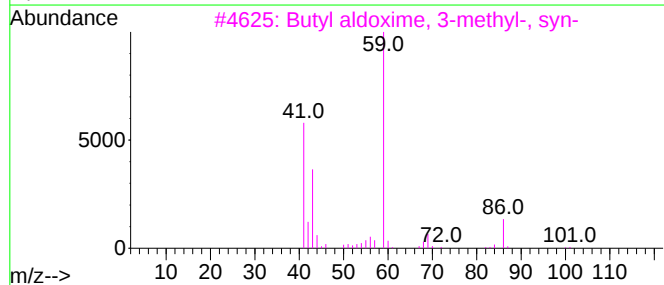
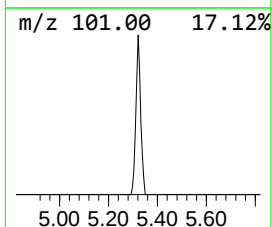
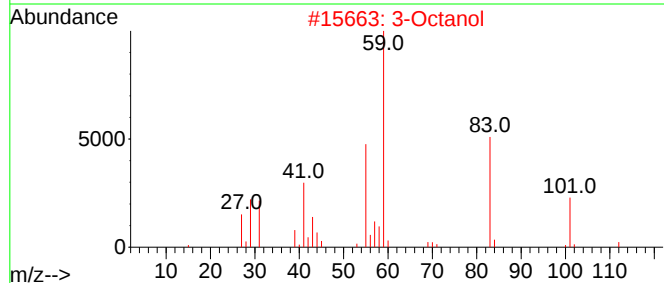
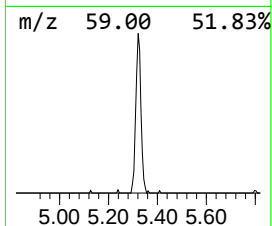
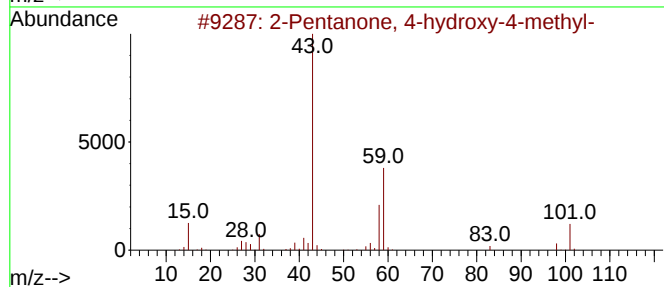
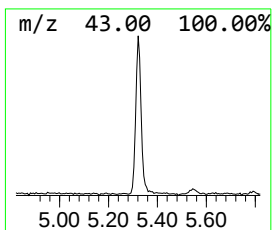
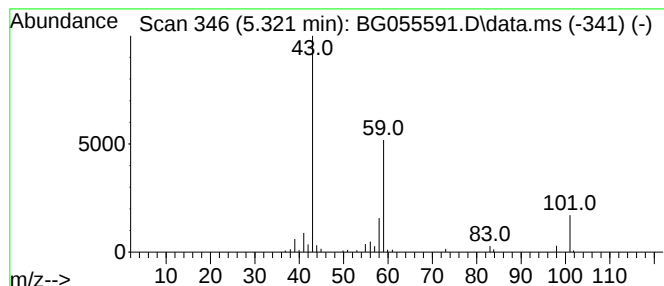
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.321	3.24 ng	77526	1,4-Dichlorobenzene-d4	8.270

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		3-Octanol	130	C8H18O	000589-98-0	33
3		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10



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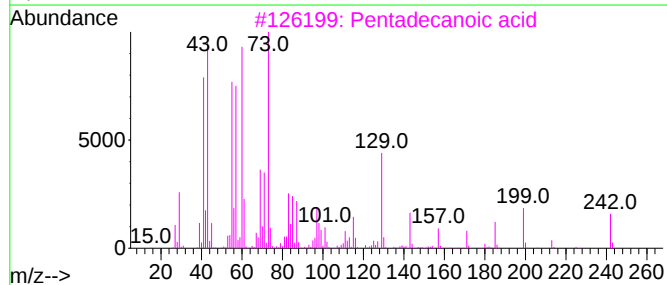
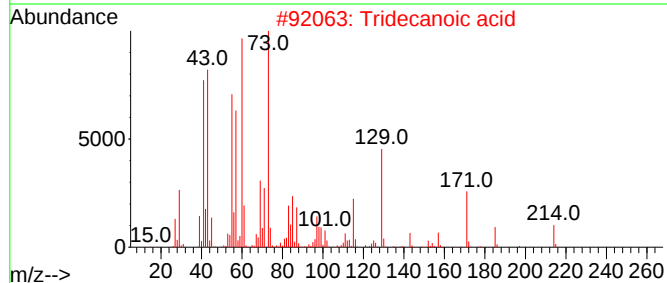
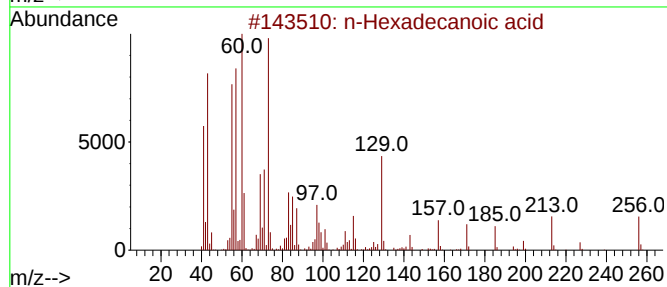
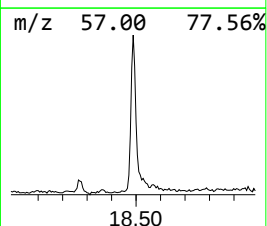
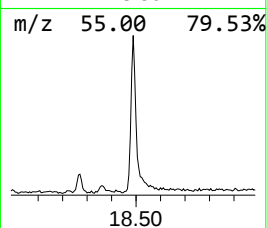
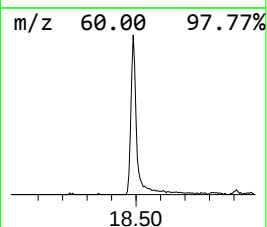
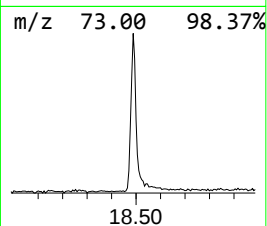
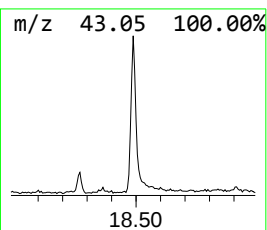
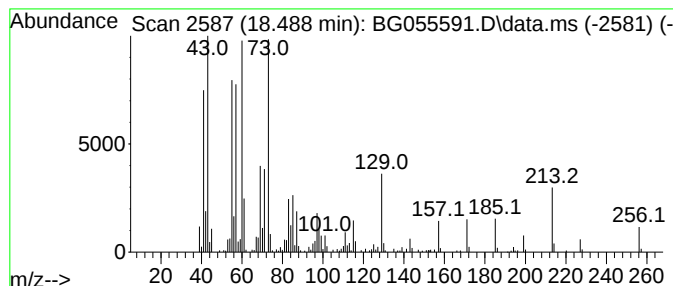
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.488	5.76 ng	408823	Phenanthrene-d10	17.630

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	92
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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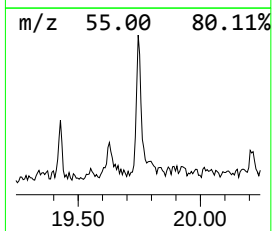
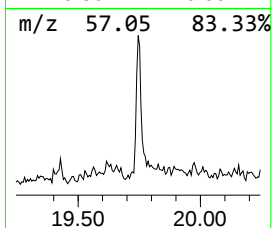
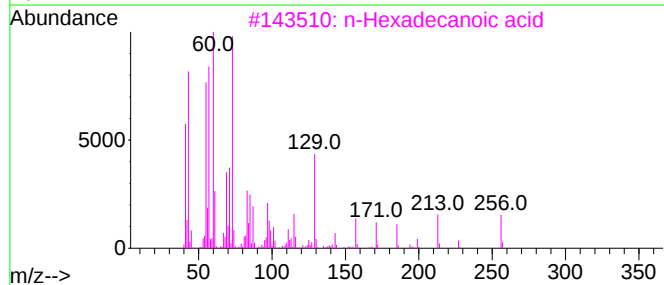
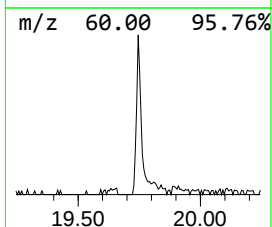
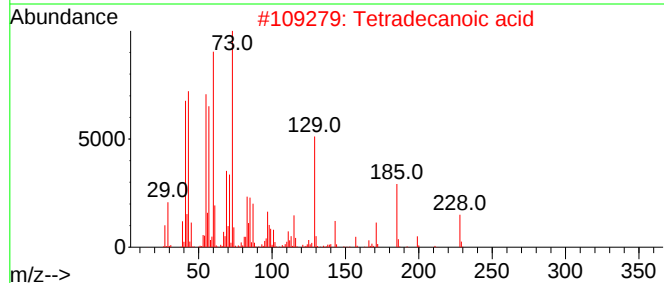
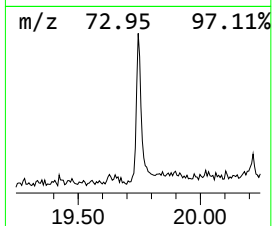
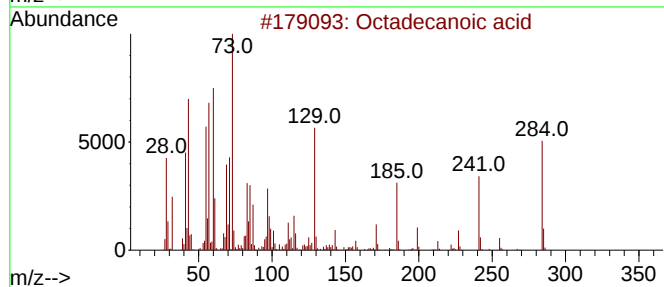
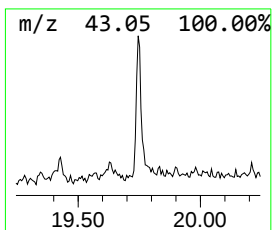
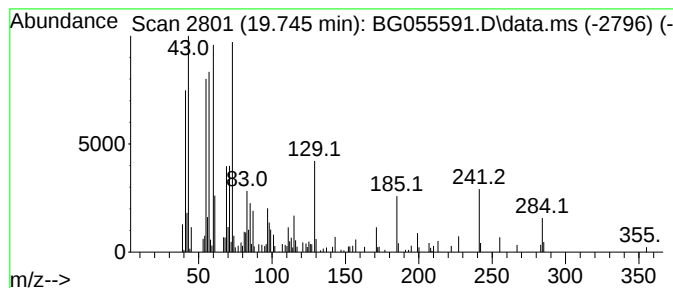
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.745	2.01 ng	142716	Phenanthrene-d10	17.630

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4			n-Decanoic acid	172	C10H20O2	000334-48-5	86
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	80



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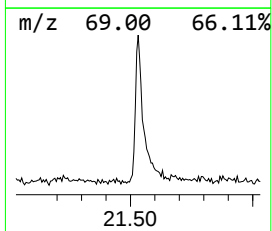
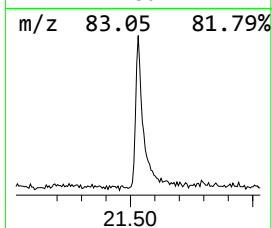
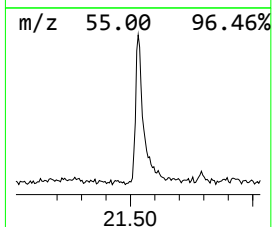
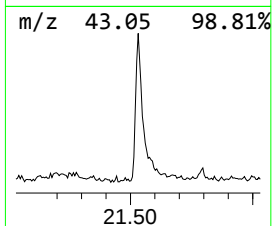
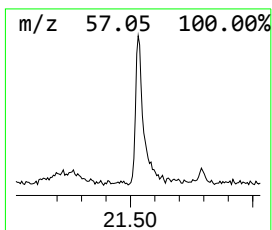
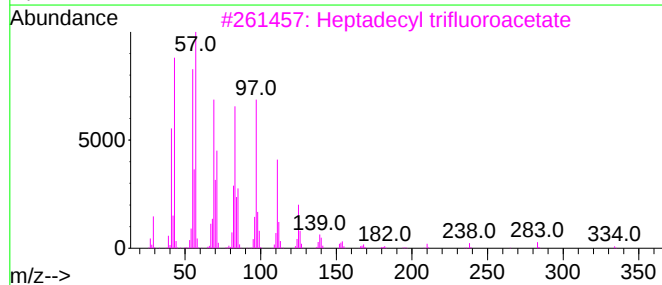
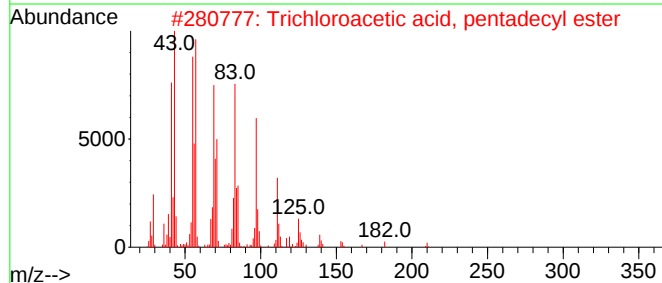
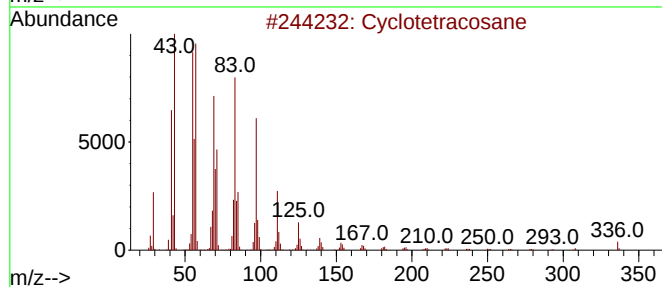
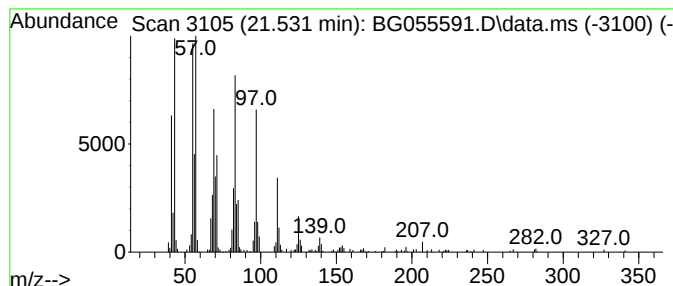
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 5 Cyclotetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.531	4.76 ng	385707	Chrysene-d12	21.925

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetracosane	336	C24H48	000297-03-0	95
2			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
3			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
4			1-Docosene	308	C22H44	001599-67-3	93
5			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.323	35.3	ng	845567	1	8.270	478692	20.0
2-Pentanone, 4-...	5.321	3.2	ng	77526	1	8.270	478692	20.0
n-Hexadecanoic ...	18.488	5.8	ng	408823	4	17.630	1419180	20.0
Octadecanoic acid	19.745	2.0	ng	142716	4	17.630	1419180	20.0
Cyclotetracosane	21.531	4.8	ng	385707	5	21.925	1621950	20.0