

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042321\
 Data File : BP005394.D
 Acq On : 23 Apr 2021 15:25
 Operator : CG/JU
 Sample : M2131-02
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 IDW-AQ-FT1-042121

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-BP042121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005394.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.234	359	365	377	rBV	276265	409404	14.86%	4.222%
2	6.822	629	635	648	rBV2	146458	336813	12.22%	3.473%
3	7.634	765	773	782	rBV	117147	177530	6.44%	1.831%
4	8.799	963	971	978	rBV	425081	697243	25.30%	7.190%
5	10.422	1239	1247	1255	rBV	122026	204703	7.43%	2.111%
6	12.916	1663	1671	1684	rBV	925073	1365605	49.55%	14.081%
7	13.763	1809	1815	1823	rBV	43770	66293	2.41%	0.684%
8	13.957	1841	1848	1861	rBV3	16902	30299	1.10%	0.312%
9	14.304	1899	1907	1917	rBV	172389	265680	9.64%	2.740%
10	15.810	2155	2163	2171	rBV	953874	1340888	48.65%	13.827%
11	16.881	2340	2345	2354	rVB	39136	53969	1.96%	0.557%
12	17.069	2370	2377	2386	rBV	244678	348924	12.66%	3.598%
13	17.975	2526	2531	2539	rBV	140890	194775	7.07%	2.008%
14	19.216	2738	2742	2753	rBV	82566	115679	4.20%	1.193%
15	19.651	2810	2816	2824	rBV	2539257	2755968	100.00%	28.418%
16	20.857	3017	3021	3023	rBV	22228	32264	1.17%	0.333%
17	20.892	3023	3027	3035	rVV3	92376	162392	5.89%	1.675%
18	20.963	3035	3039	3046	rVB	77628	99821	3.62%	1.029%
19	21.175	3070	3075	3080	rBV	416214	517632	18.78%	5.338%
20	23.433	3453	3459	3466	rVB	287411	522008	18.94%	5.383%

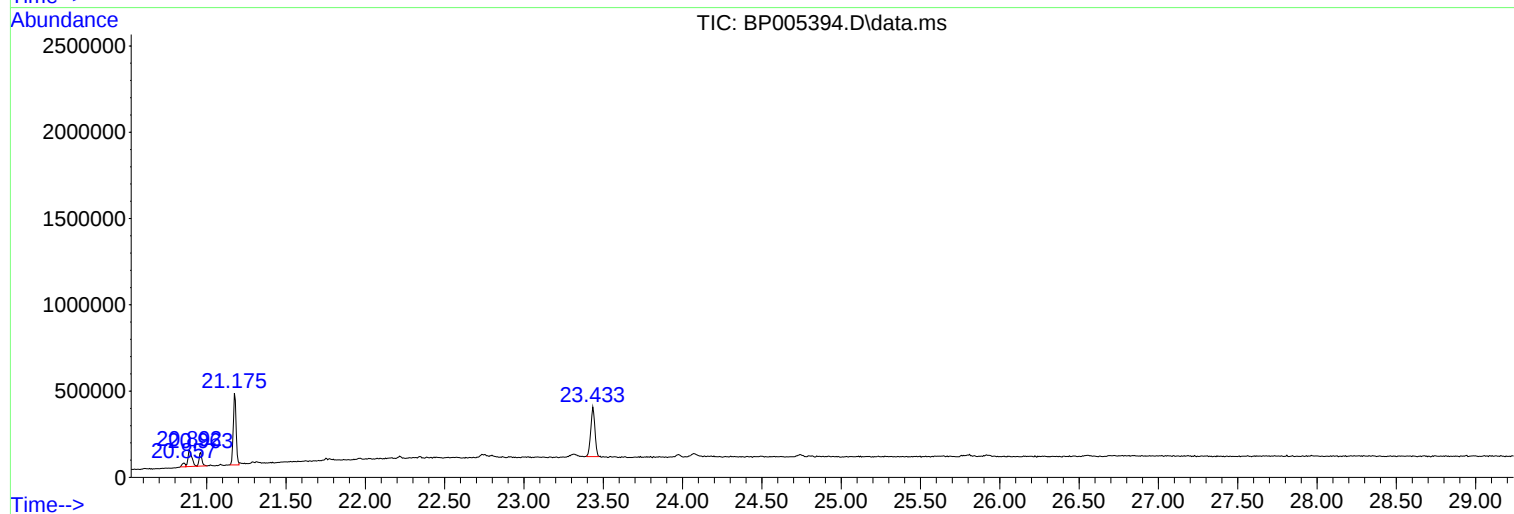
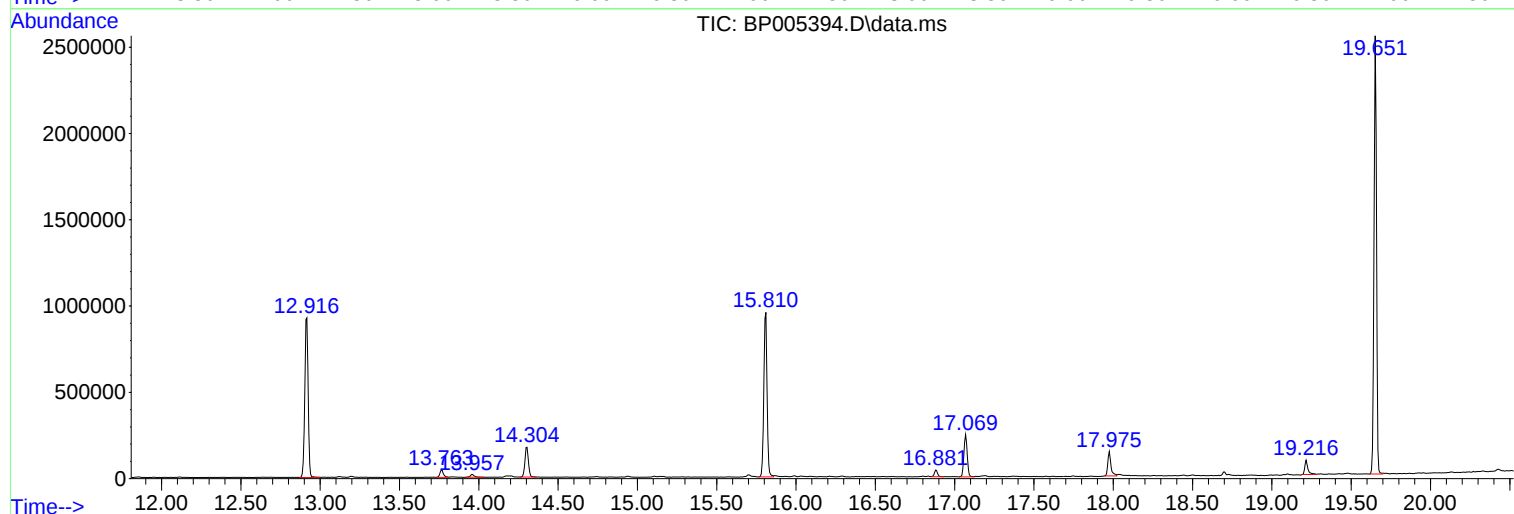
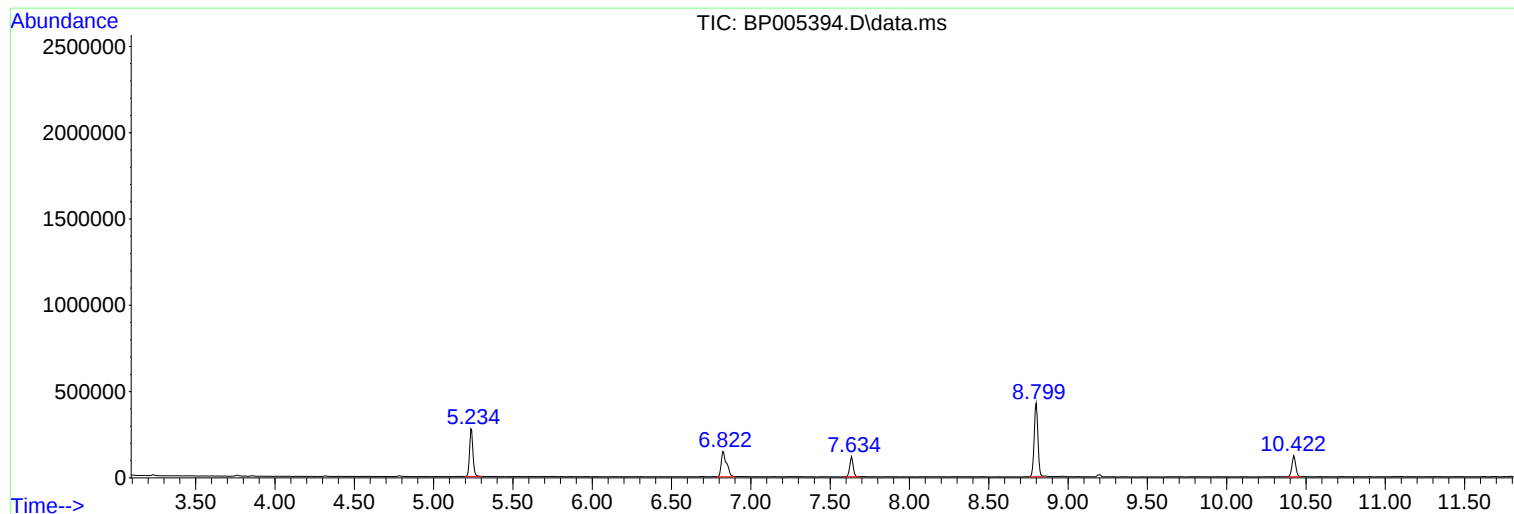
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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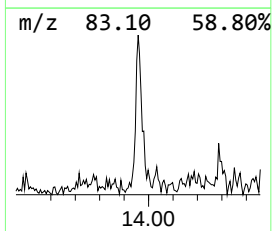
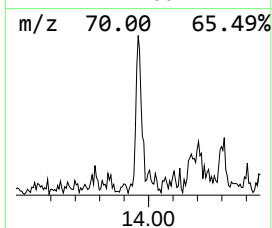
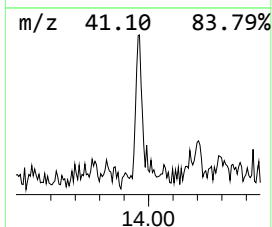
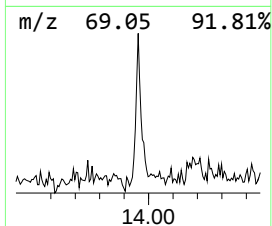
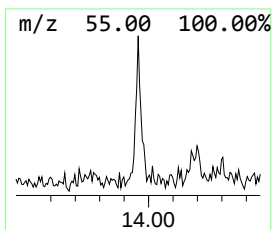
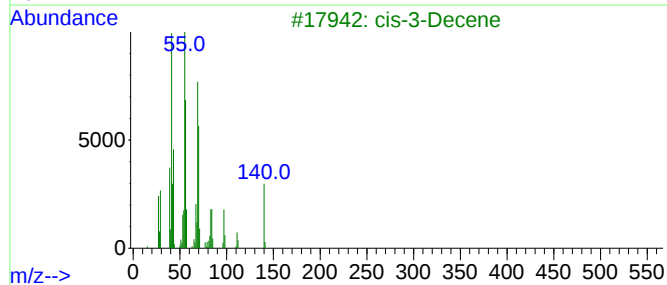
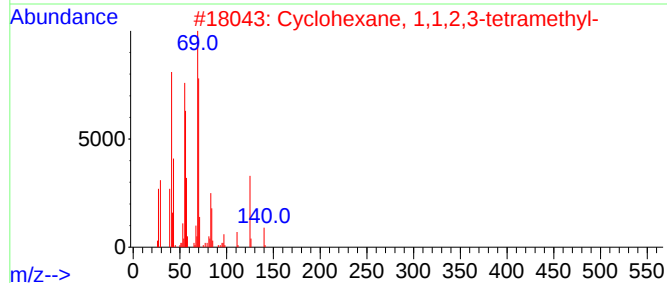
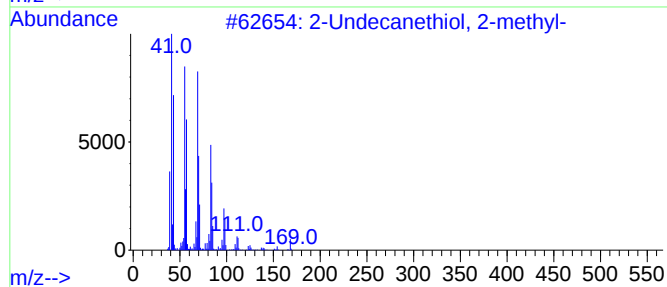
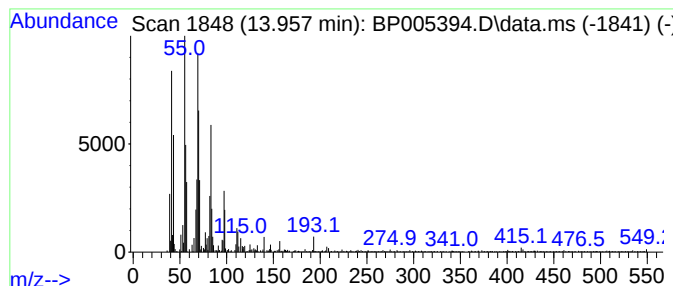
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Undecanethiol, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.957	2.28 ng	30299	Acenaphthene-d10	14.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Undecanethiol, 2-methyl-	202	C12H26S	010059-13-9	72
2			Cyclohexane, 1,1,2,3-tetramethyl-	140	C10H20	006783-92-2	64
3			cis-3-Decene	140	C10H20	019398-86-8	62
4			3-Octene, 4-ethyl-	140	C10H20	053966-51-1	52
5			4-Octene, 2,6-dimethyl-, [S-(Z)]-	140	C10H20	062960-77-4	52



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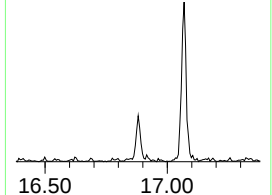
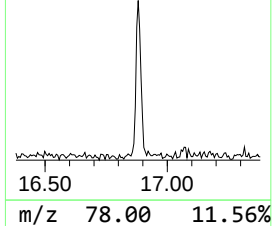
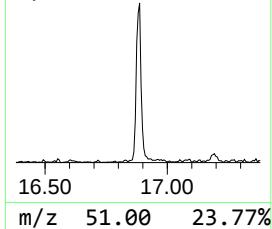
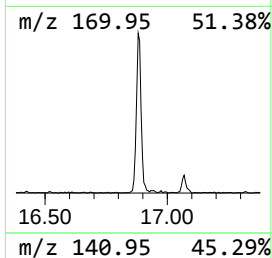
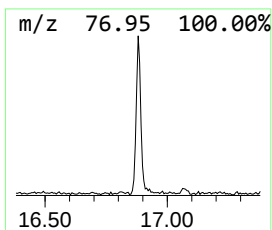
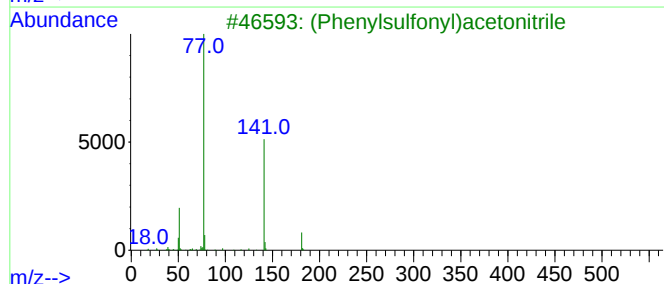
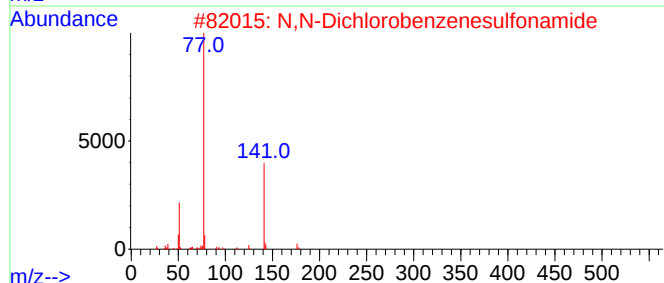
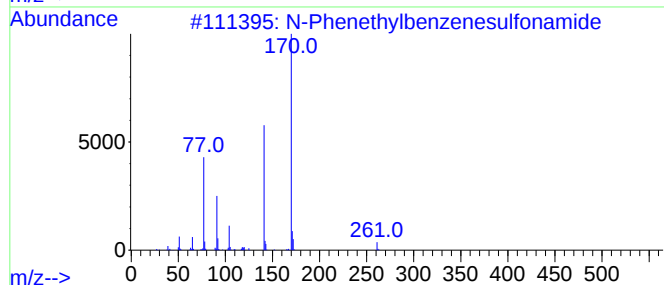
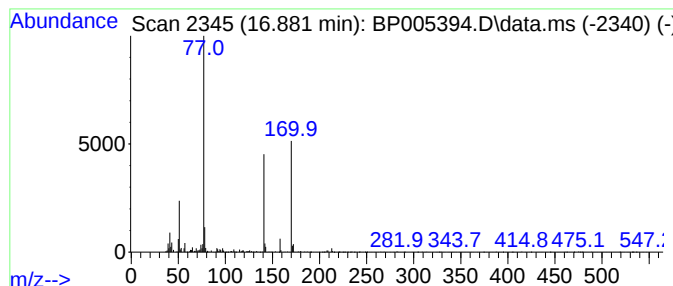
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 N-Phenethylbenzenesulfonamide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.881	3.09 ng	53969	Phenanthrene-d10	17.069

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-Phenethylbenzenesulfonamide	261	C14H15NO2S	077198-99-3	74
2			N,N-Dichlorobenzenesulfonamide	225	C6H5Cl2NO2S	000473-29-0	59
3			(Phenylsulfonyl)acetonitrile	181	C8H7NO2S	007605-28-9	59
4			Propanedinitrile, [1-phenyl-2-(p...	308	C17H12N2O2S	136289-43-5	53
5			Benzenesulfonamide, N-butyl-	213	C10H15NO2S	003622-84-2	50



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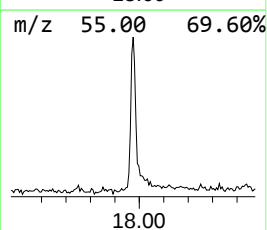
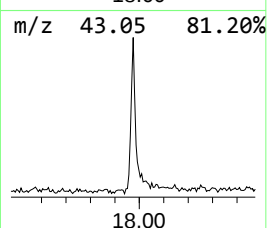
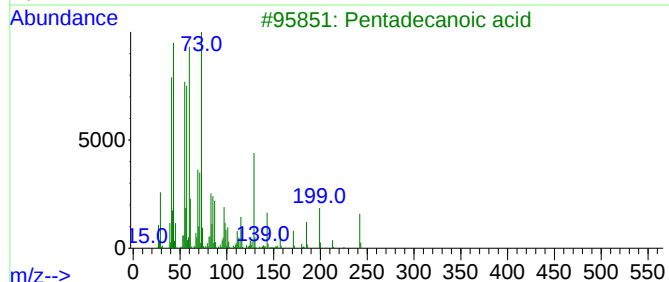
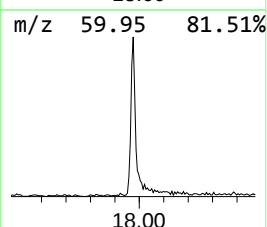
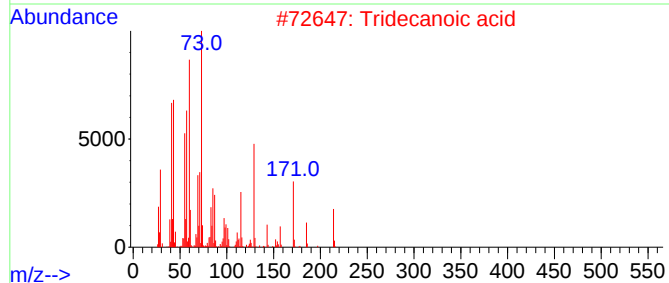
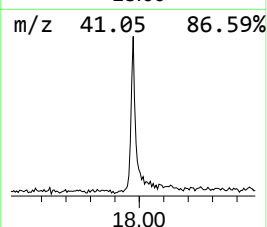
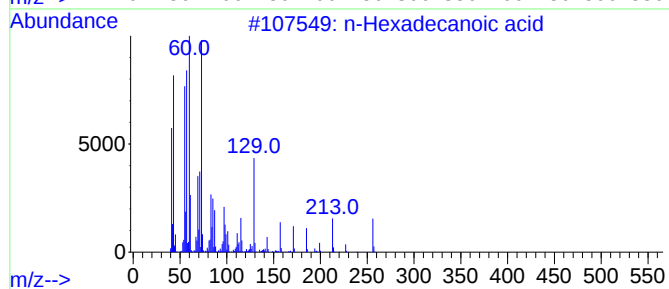
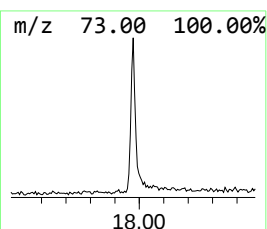
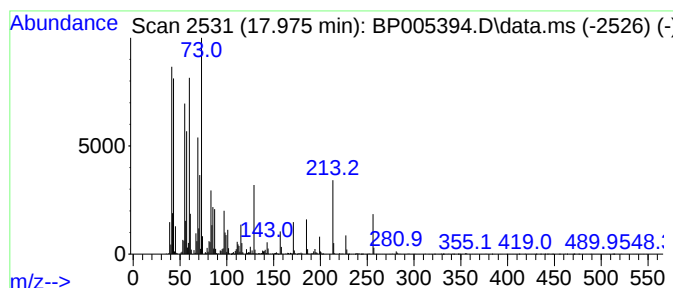
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
17.975	11.16 ng	194775	Phenanthrene-d10		17.069	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	93
2	Tridecanoic acid		214	C13H26O2	000638-53-9	92
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	87
4	Undecanoic acid		186	C11H22O2	000112-37-8	58
5	Tetradecanoic acid		228	C14H28O2	000544-63-8	53



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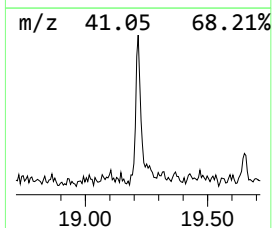
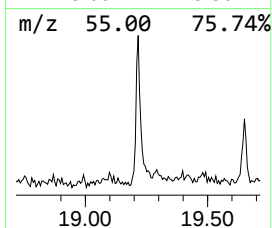
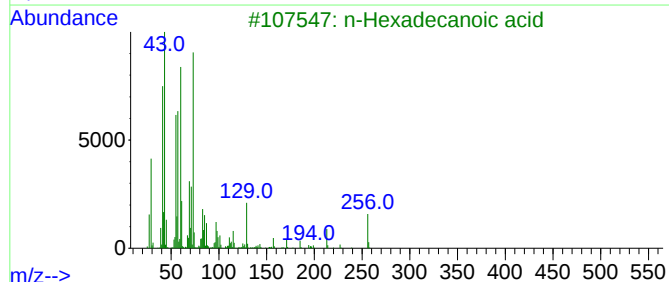
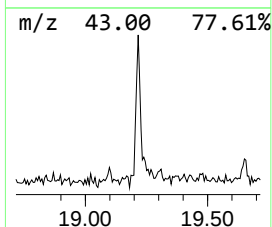
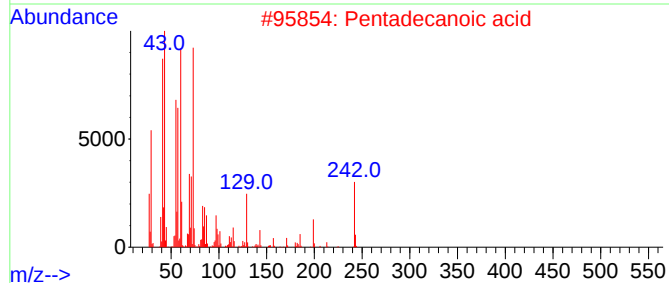
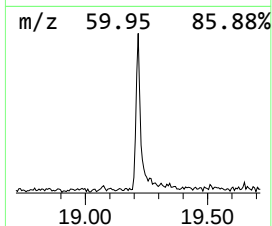
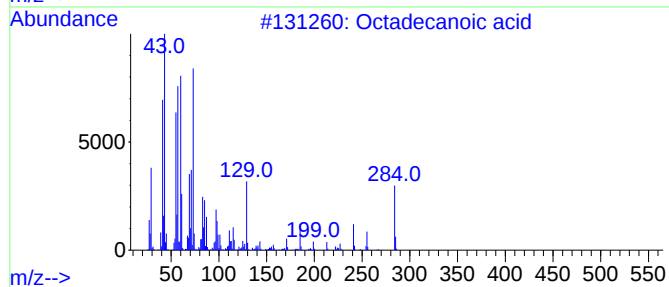
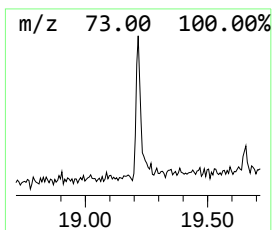
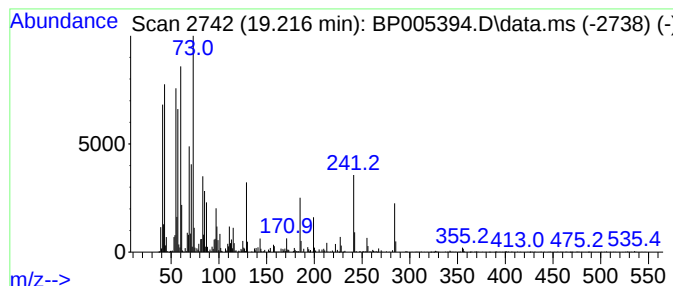
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.216	4.47 ng	115679	Chrysene-d12	21.174

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	93
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5			Tridecanoic acid	214	C13H26O2	000638-53-9	53



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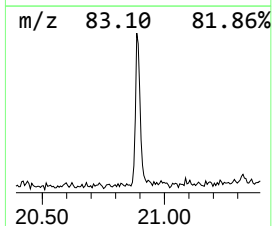
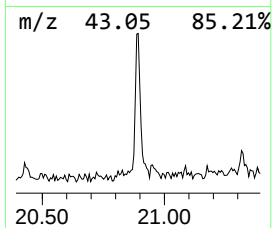
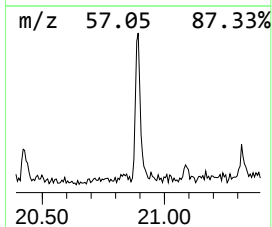
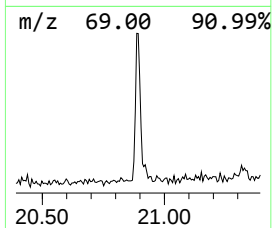
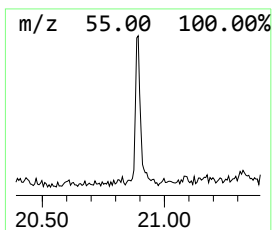
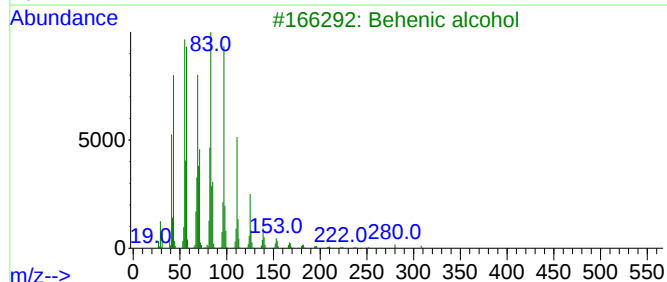
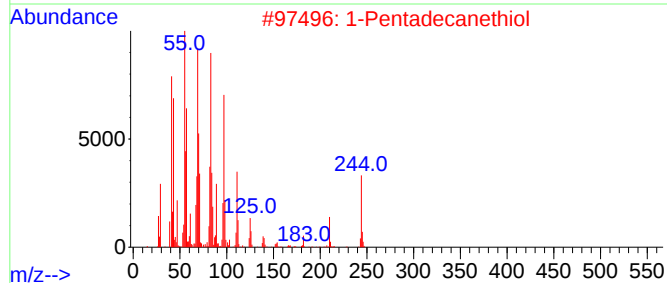
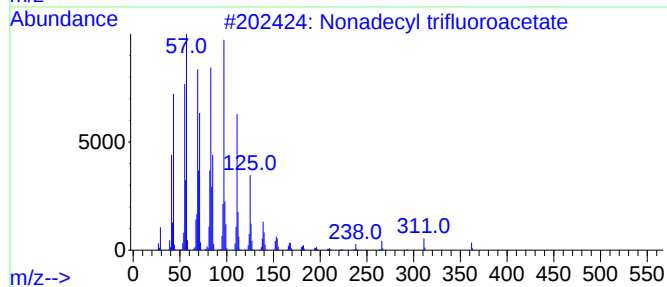
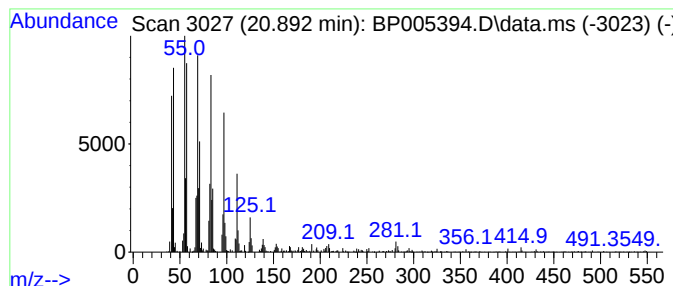
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Nonadecyl trifluoroacetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.892	6.27 ng	162392	Chrysene-d12	21.174

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
2			1-Pentadecanethiol	244	C15H32S	025276-70-4	91
3			Behenic alcohol	326	C22H46O	000661-19-8	91
4			1-Heptacosanol	396	C27H56O	002004-39-9	89
5			Octacosanol	410	C28H58O	000557-61-9	86



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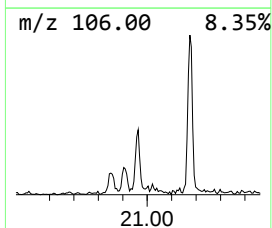
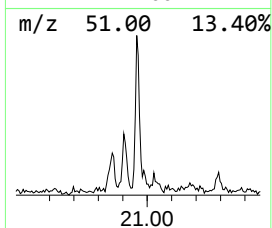
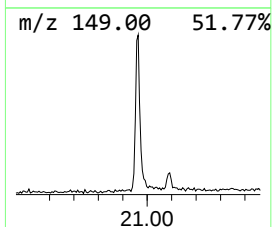
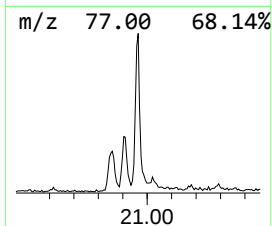
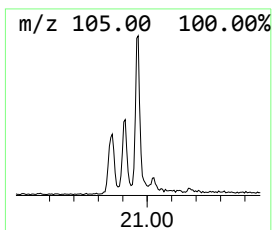
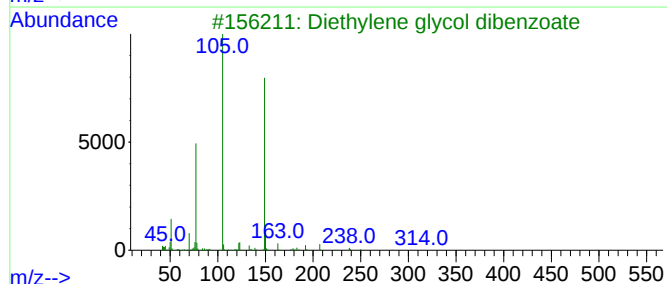
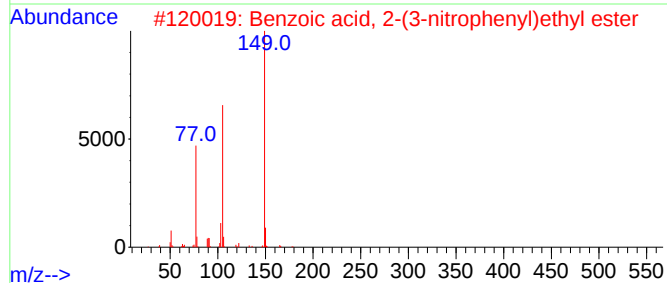
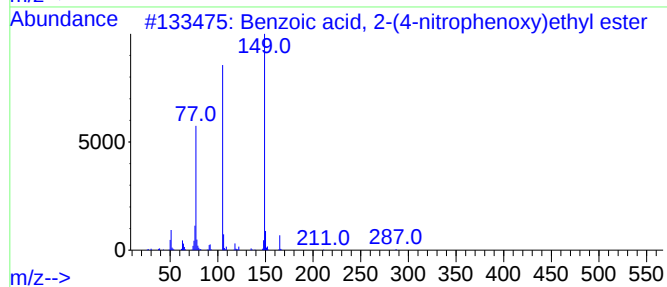
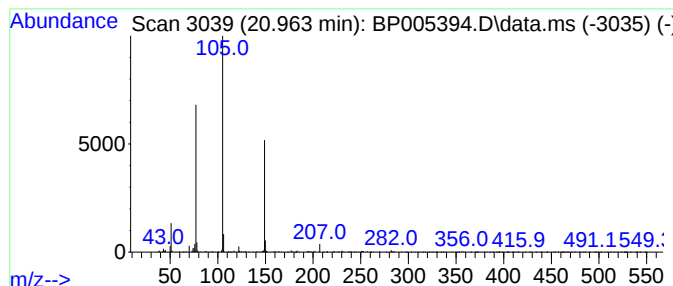
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzoic acid, 2-(4-nitrophe... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.963	3.86 ng	99821	Chrysene-d12	21.174

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	72
2			Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	72
3			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	53
4			Vinyl benzoate	148	C9H8O2	000769-78-8	49
5			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042321\
Data File : BP005394.D
Acq On : 23 Apr 2021 15:25
Operator : CG/JU
Sample : M2131-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
IDW-AQ-FT1-042121

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Undecanethiol...	13.957	2.3	ng	30299	3	14.298	265680	20.0
N-Phenethylbenz...	16.881	3.1	ng	53969	4	17.069	348924	20.0
n-Hexadecanoic ...	17.975	11.2	ng	194775	4	17.069	348924	20.0
Octadecanoic acid	19.216	4.5	ng	115679	5	21.174	517632	20.0
Nonadecyl trifl...	20.892	6.3	ng	162392	5	21.174	517632	20.0
Benzoic acid, 2...	20.963	3.9	ng	99821	5	21.174	517632	20.0