

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF063022\
 Data File : BF129069.D
 Acq On : 30 Jun 2022 20:30
 Operator : CG\JU
 Sample : N3434-06
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B2205-35

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_F\Methods\8270-BF062922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129069.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.363	4	13	22	rVB	3302497	4458900	35.98%	5.162%
2	5.593	556	562	565	rBV	9818697	10455882	84.36%	12.105%
3	6.581	723	730	733	rBV	8639321	10567821	85.27%	12.234%
4	6.957	790	794	797	rVB	2632261	2339101	18.87%	2.708%
5	7.522	883	890	893	rBV	6611311	7029402	56.72%	8.138%
6	8.239	1006	1012	1015	rBV	3442550	3110503	25.10%	3.601%
7	9.316	1188	1195	1198	rBV	12291105	12393973	100.00%	14.349%
8	9.998	1305	1311	1314	rBV	4092339	3475098	28.04%	4.023%
9	10.792	1438	1446	1449	rBV	8680532	8203366	66.19%	9.497%
10	11.492	1558	1565	1568	rBV	3892416	3543204	28.59%	4.102%
11	12.004	1646	1652	1664	rBV	666629	714624	5.77%	0.827%
12	12.792	1782	1786	1795	rBV	195570	221297	1.79%	0.256%
13	13.080	1830	1835	1839	rBV	11505443	12115815	97.76%	14.027%
14	13.557	1910	1916	1921	rBV	519538	556877	4.49%	0.645%
15	14.016	1989	1994	2007	rBV	605769	1291699	10.42%	1.495%
16	14.139	2011	2015	2018	rBV	3306348	2737375	22.09%	3.169%
17	14.233	2025	2031	2037	rBV	588392	683995	5.52%	0.792%
18	14.904	2141	2145	2152	rBV2	192676	292497	2.36%	0.339%
19	15.663	2268	2274	2281	rBV	1709189	2186571	17.64%	2.531%

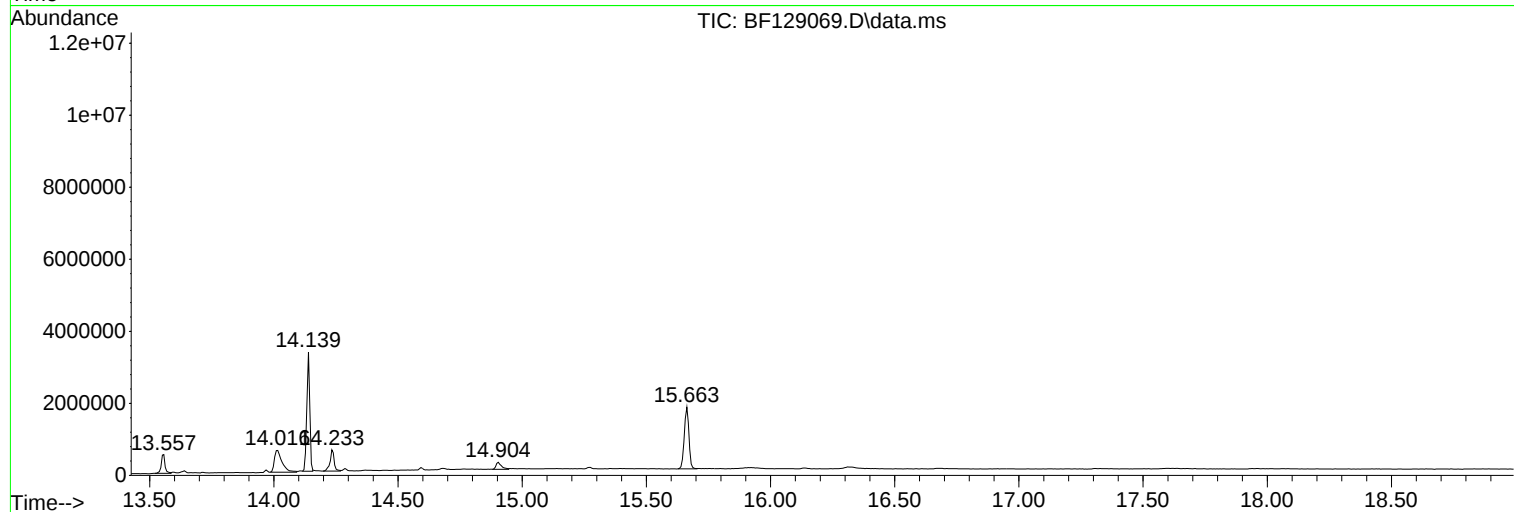
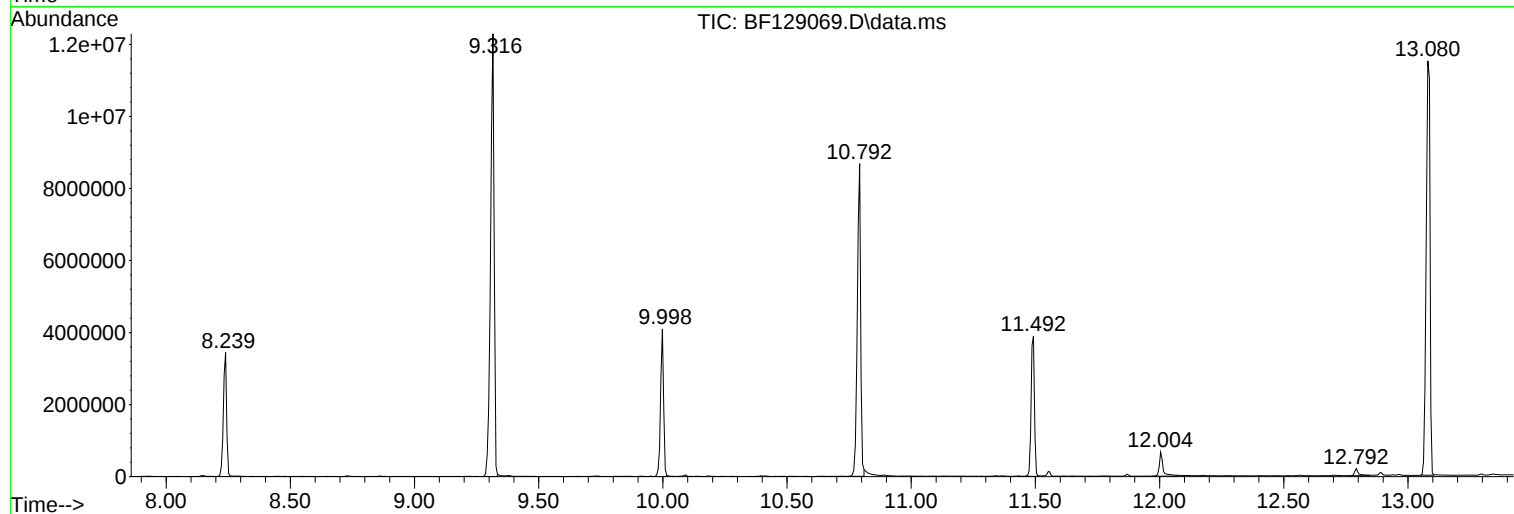
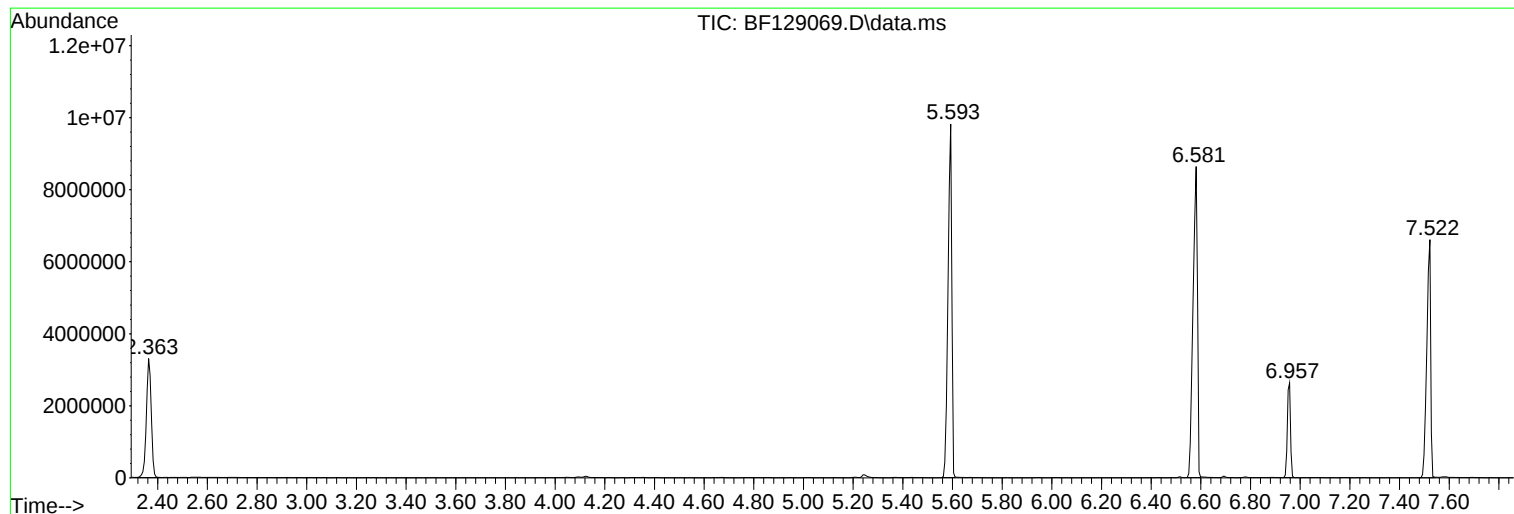
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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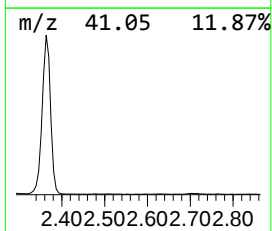
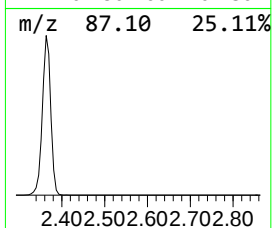
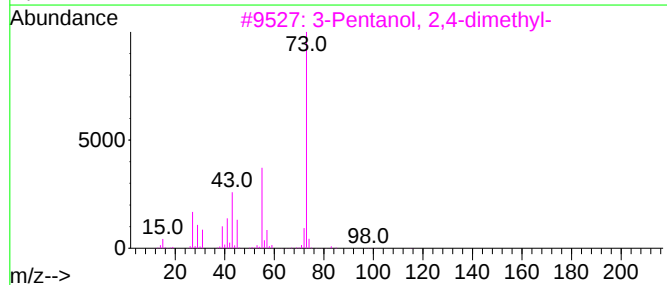
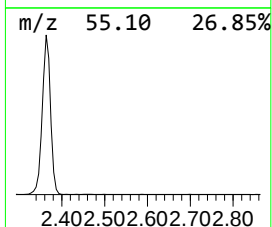
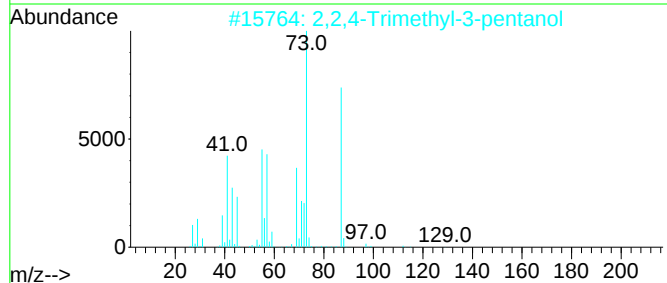
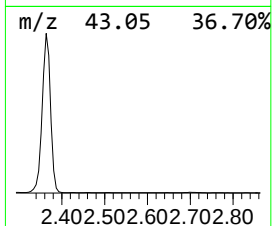
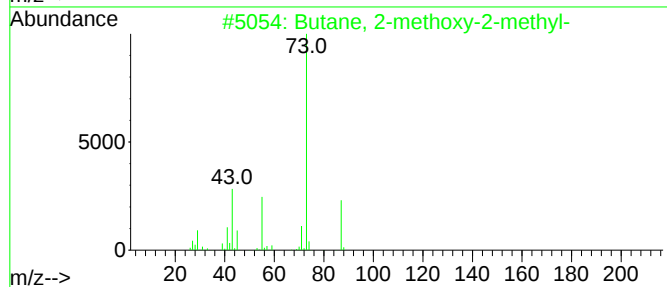
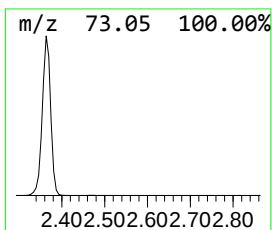
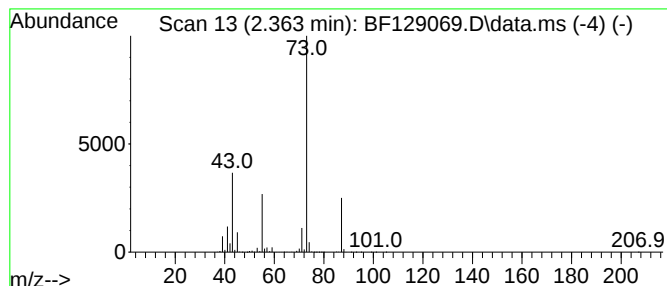
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.363	38.12 ng	4458900	1,4-Dichlorobenzene-d4	6.957

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	40
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22



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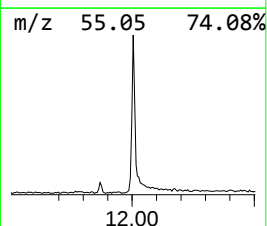
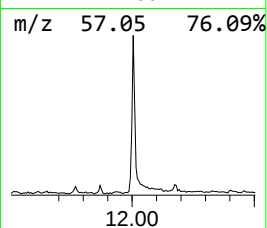
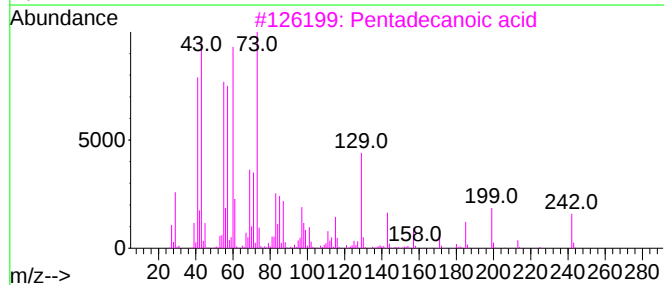
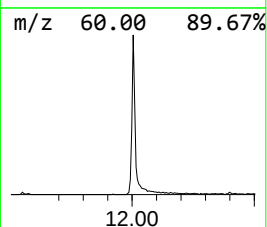
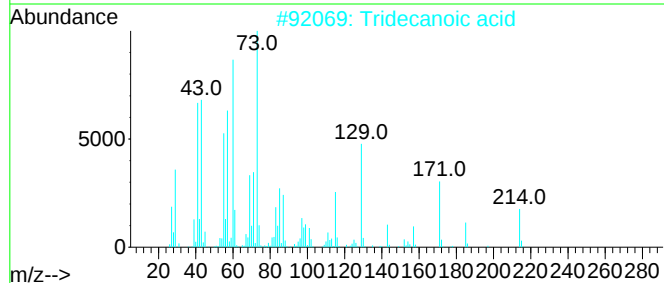
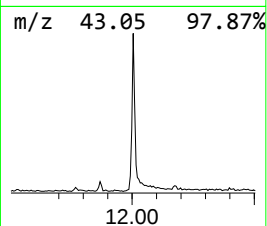
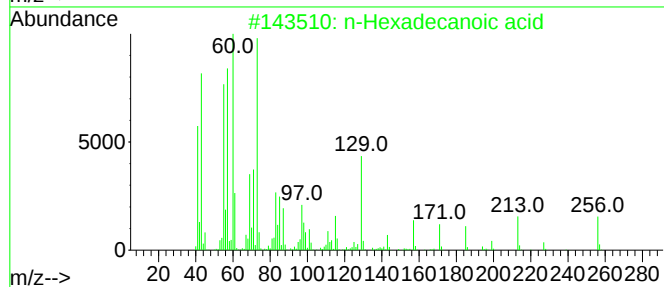
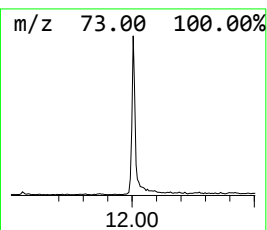
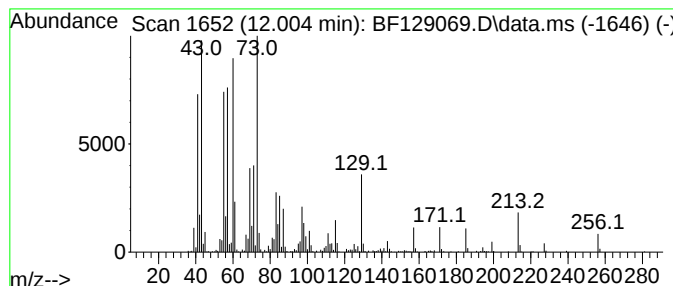
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.004	4.03 ng	714624	Phenanthrene-d10	11.492

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	95
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	94
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5		8-Methylnonanoic acid	172	C10H20O2	005963-14-4	64



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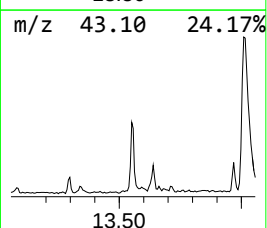
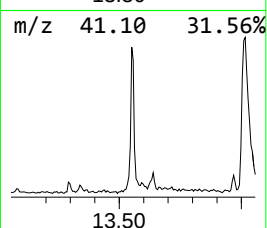
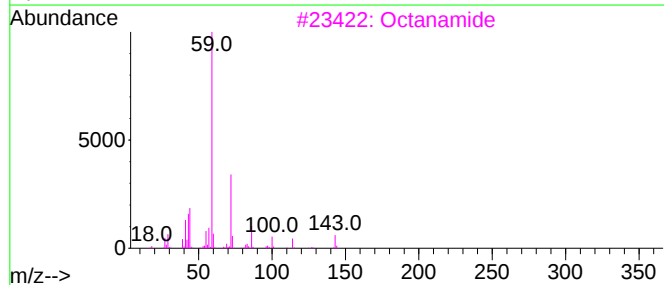
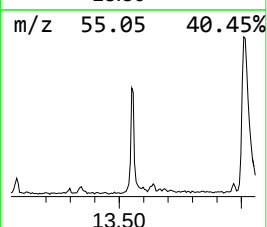
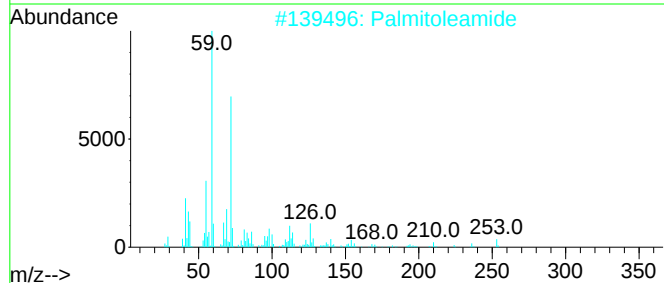
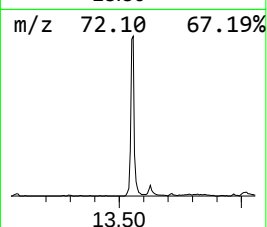
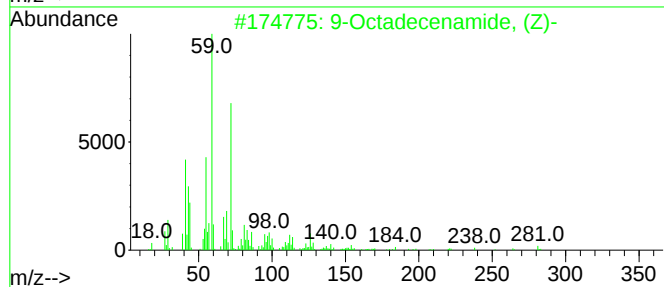
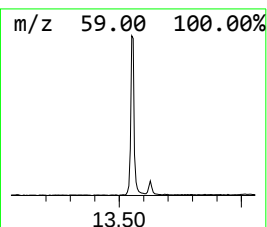
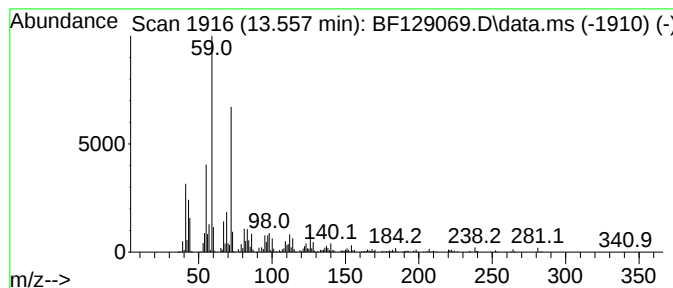
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Peak Number 3 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.557	4.07 ng	556877	Chrysene-d12	14.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99
2			Palmitoleamide	253	C16H31NO	106010-22-4	91
3			Octanamide	143	C8H17NO	000629-01-6	64
4			Hexadecanamide	255	C16H33NO	000629-54-9	59
5			Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	53



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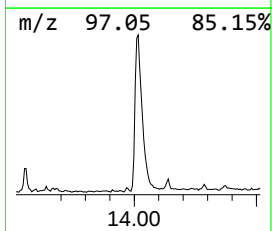
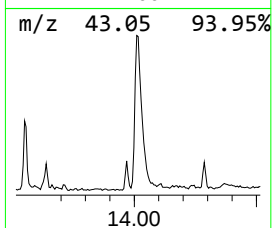
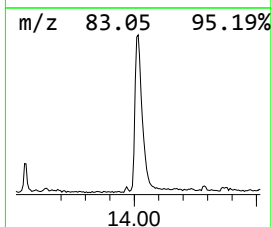
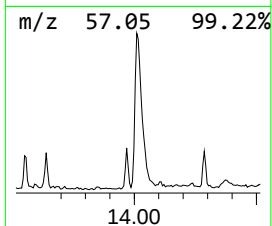
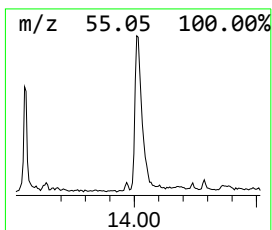
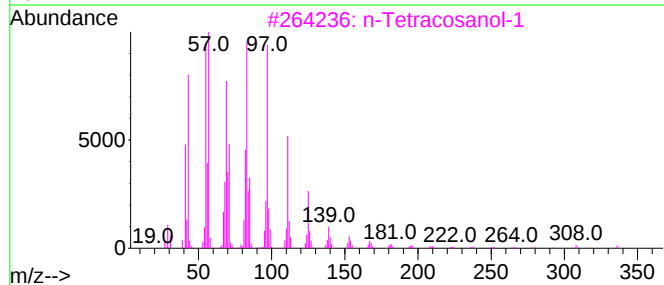
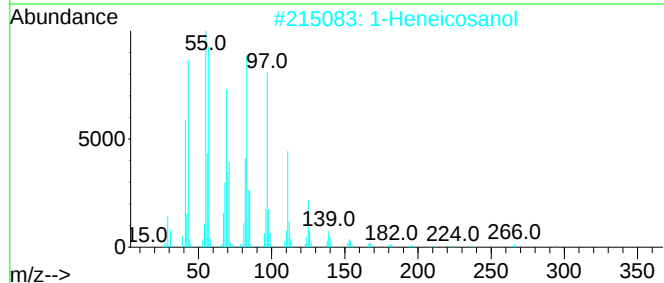
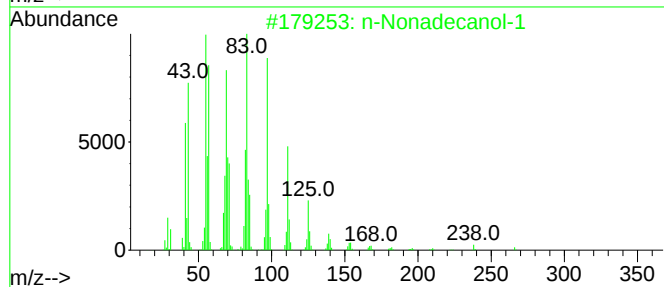
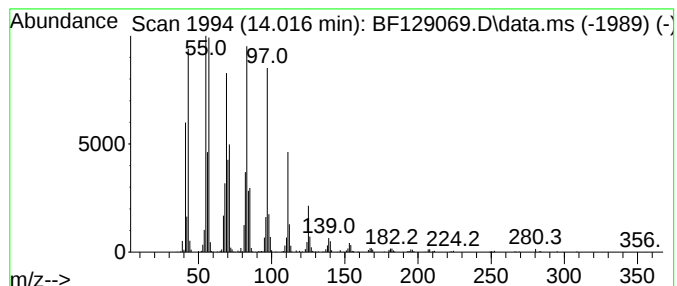
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Peak Number 4 n-Nonadecanol-1 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.016	9.44 ng	1291700	Chrysene-d12	14.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Nonadecanol-1	284	C19H40O	001454-84-8	94
2			1-Heneicosanol	312	C21H44O	015594-90-8	94
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93



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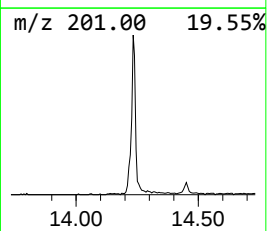
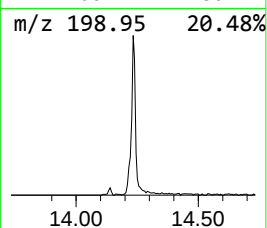
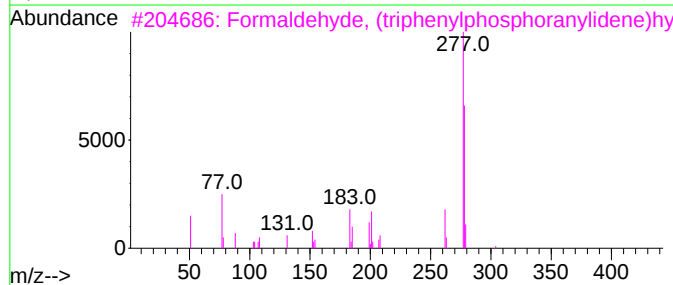
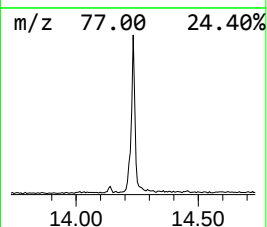
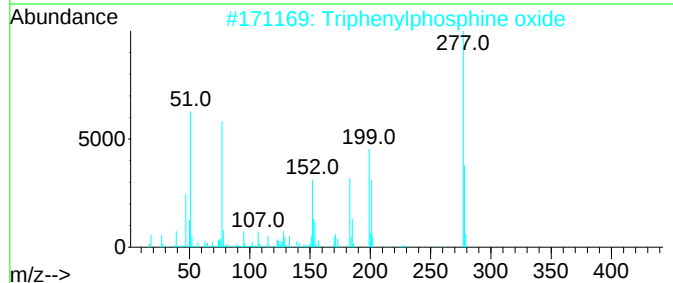
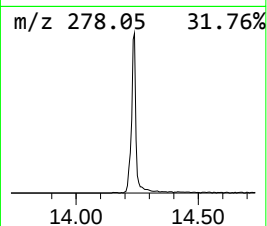
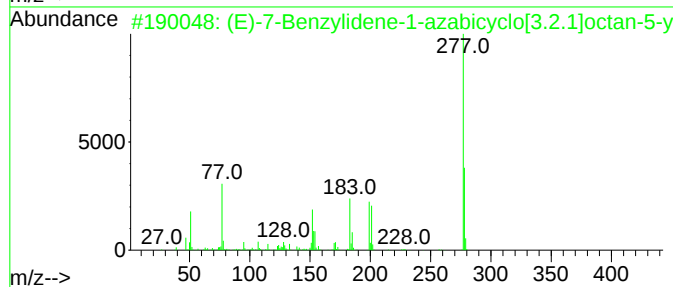
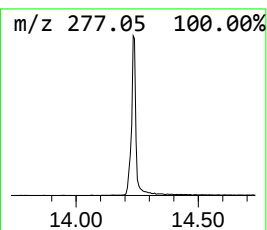
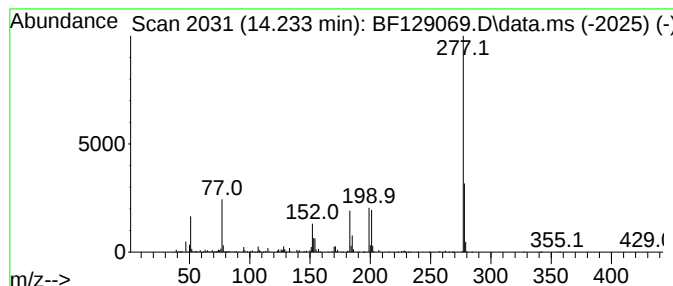
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TIC Integration Parameters: LSCINT.P

Peak Number 5 (E)-7-Benzylidene-1-azabicyclo... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.233	5.00 ng	683995	Chrysene-d12	14.139	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91
2	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	91
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
4	Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	17
5	[1,2,4]Triazolo[1,5-a]pyrimidine...	278	C15H14N6	1000350-69-0	9



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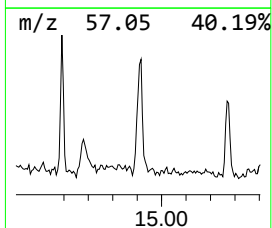
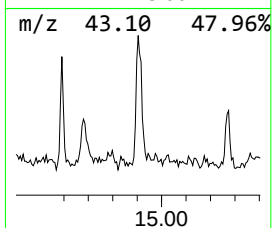
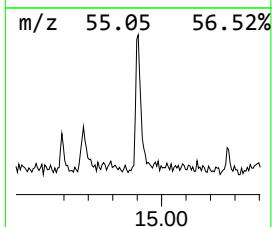
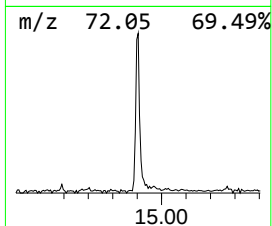
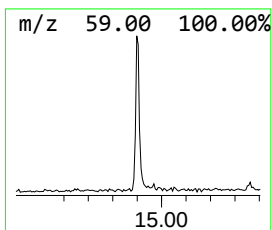
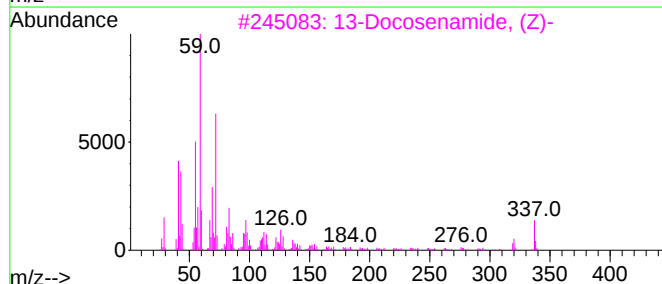
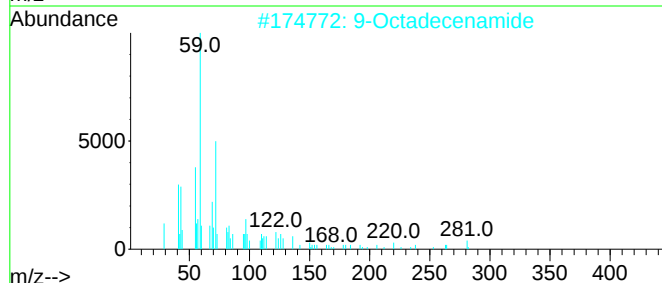
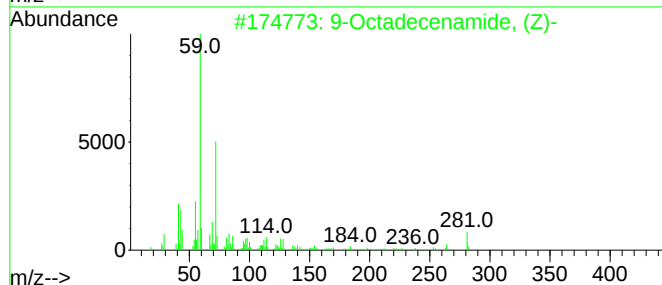
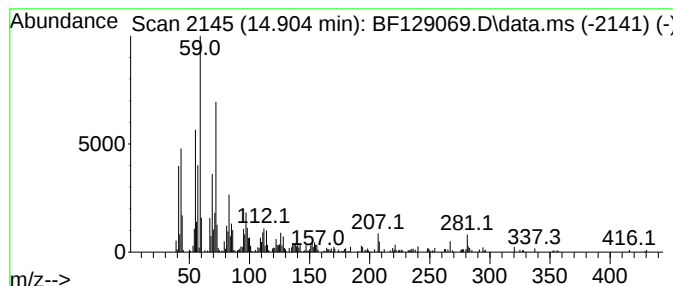
Instrument :
BNA_F
ClientSampleId :
B2205-35

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-Octadecenamide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.904	2.68 ng	292497	Perylene-d12	15.663	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	96
2	9-Octadecenamide	281	C18H35NO	003322-62-1	87
3	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	86
4	Palmitoleamide	253	C16H31NO	106010-22-4	72
5	Dodecanamide	199	C12H25NO	001120-16-7	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF063022\
Data File : BF129069.D
Acq On : 30 Jun 2022 20:30
Operator : CG\JU
Sample : N3434-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B2205-35

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT 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
Butane, 2-metho...	2.363	38.1	ng	4458900	1	6.957	2339100	20.0
n-Hexadecanoic ...	12.004	4.0	ng	714624	4	11.492	3543200	20.0
9-Octadecenamid...	13.557	4.1	ng	556877	5	14.139	2737380	20.0
n-Nonadecanol-1	14.016	9.4	ng	1291700	5	14.139	2737380	20.0
(E)-7-Benzylide...	14.233	5.0	ng	683995	5	14.139	2737380	20.0
9-Octadecenamide	14.904	2.7	ng	292497	6	15.663	2186570	20.0