

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
 Data File : BF128525.D
 Acq On : 27 May 2022 23:00
 Operator : CG\JU
 Sample : N2921-02
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P013-SS002-0612-01

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-BF052622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128525.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.081	471	475	482	rVB	105284	143420	2.40%	0.351%
2	5.457	533	539	542	rBV	4569116	5084266	85.19%	12.431%
3	6.463	703	710	713	rBV	4422729	5175805	86.72%	12.654%
4	6.575	726	729	738	rBV	114508	102665	1.72%	0.251%
5	6.839	770	774	777	rBV	1657361	1449786	24.29%	3.545%
6	7.398	863	869	872	rBV	3211467	3611980	60.52%	8.831%
7	8.122	986	992	995	rBV	1968309	1885960	31.60%	4.611%
8	9.198	1169	1175	1178	rBV	6366568	5968143	100.00%	14.592%
9	9.280	1185	1189	1194	rVB2	69853	71488	1.20%	0.175%
10	9.875	1284	1290	1294	rBV	2316803	2012008	33.71%	4.919%
11	10.663	1418	1424	1427	rBV	3463267	3173264	53.17%	7.758%
12	10.786	1442	1445	1450	rVB2	47471	70211	1.18%	0.172%
13	11.363	1539	1543	1546	rBV	2220338	1844538	30.91%	4.510%
14	11.892	1629	1633	1638	rBV	600494	576896	9.67%	1.410%
15	12.604	1751	1754	1763	rVB	320892	321855	5.39%	0.787%
16	12.680	1763	1767	1776	rBV	593122	645836	10.82%	1.579%
17	12.951	1809	1813	1817	rBV	4403020	4427888	74.19%	10.826%
18	13.892	1969	1973	1983	rVB3	200886	411954	6.90%	1.007%
19	14.004	1988	1992	1995	rBV	1268432	1189111	19.92%	2.907%
20	14.104	2003	2009	2013	rVB	1049916	1130250	18.94%	2.763%
21	14.180	2020	2022	2025	rVB	79893	61274	1.03%	0.150%
22	15.468	2236	2241	2245	rVB	887304	1073056	17.98%	2.624%
23	16.086	2342	2346	2354	rVB5	63298	142610	2.39%	0.349%
24	17.292	2547	2551	2557	rVB4	167806	326780	5.48%	0.799%

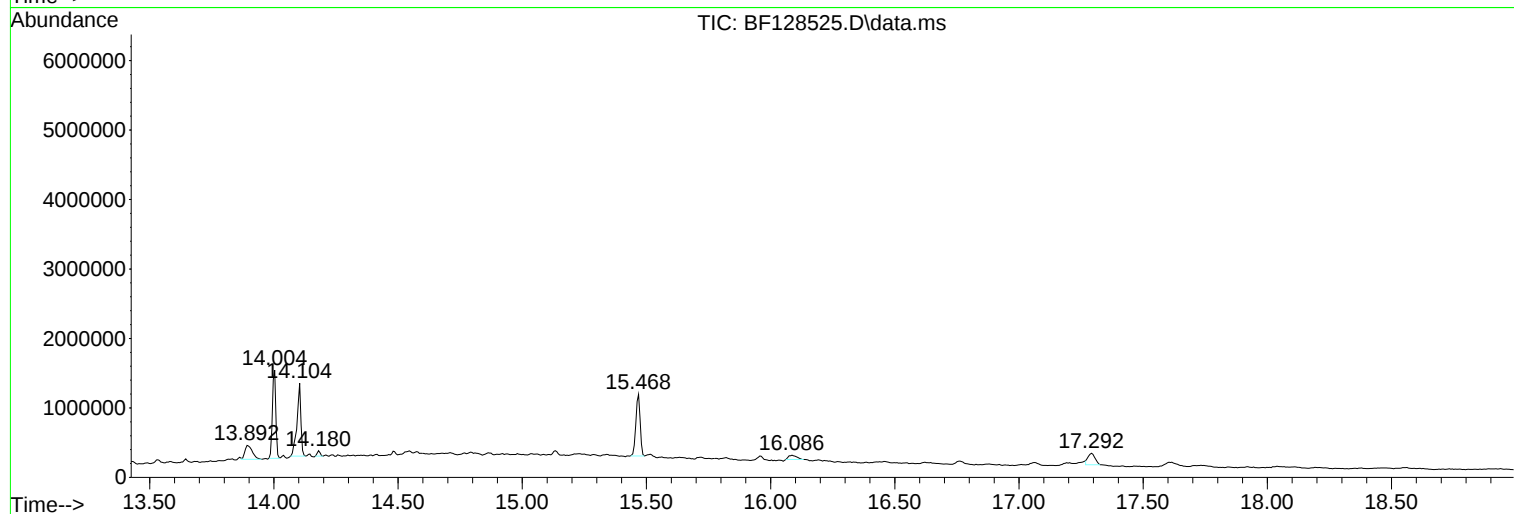
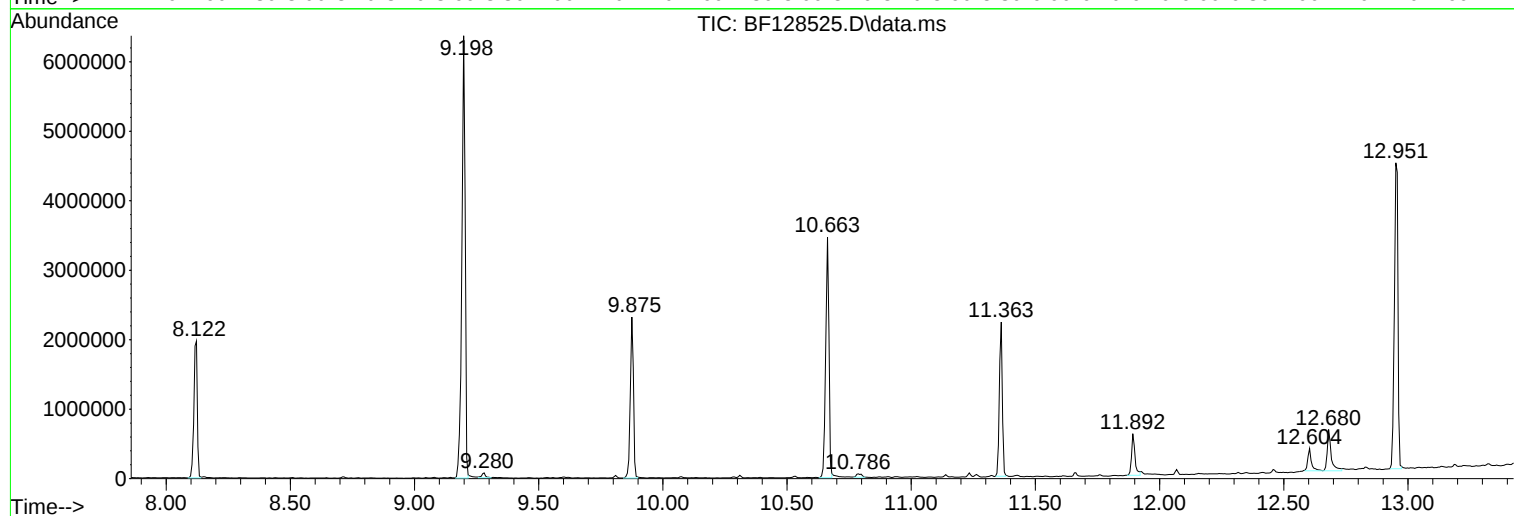
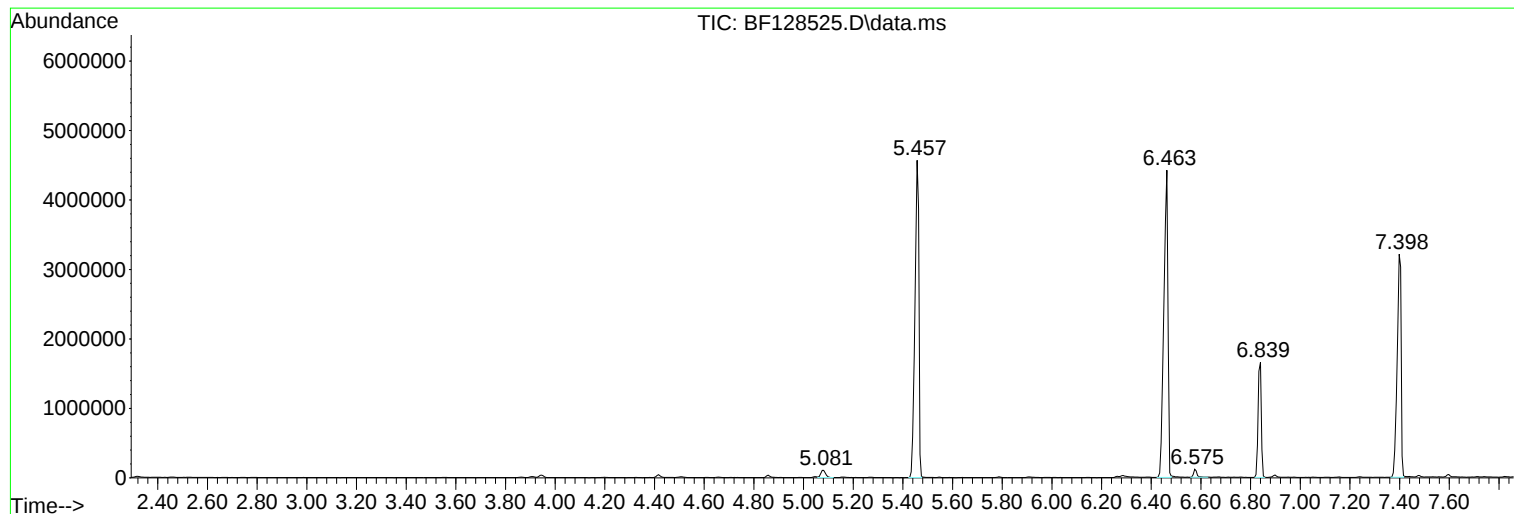
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ClientSampleId :
P013-SS002-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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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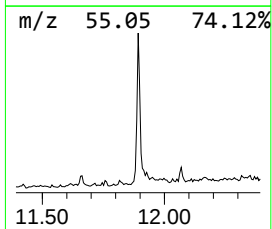
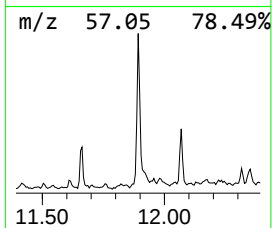
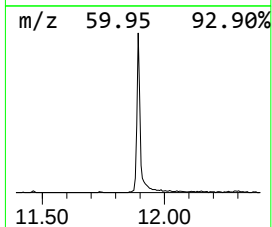
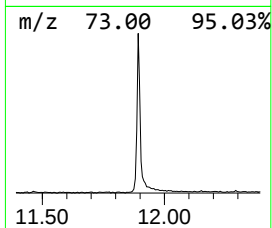
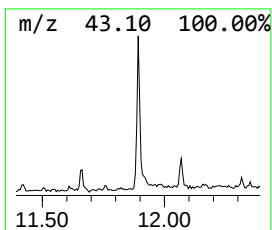
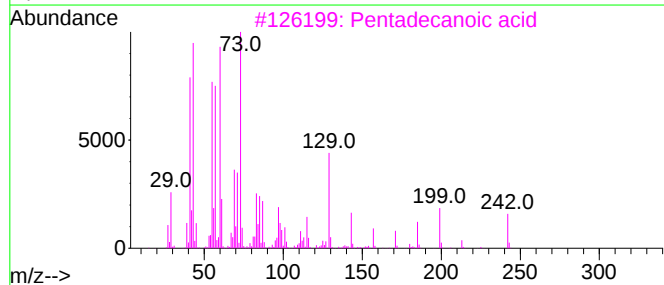
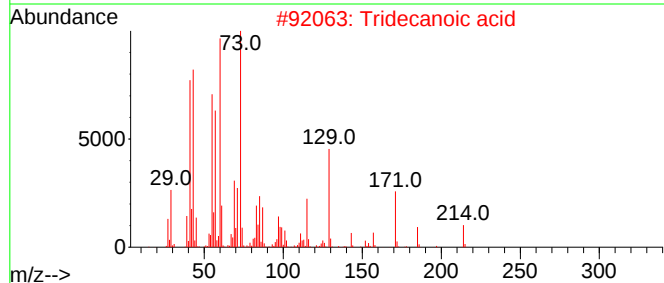
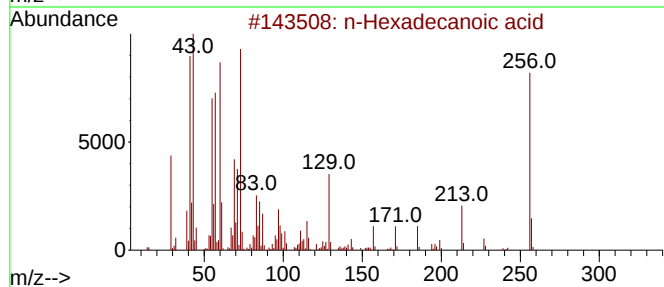
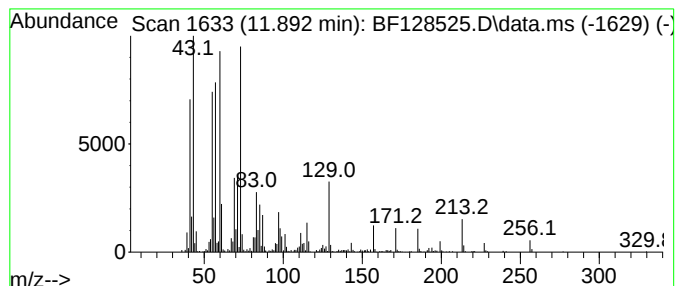
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	6.26 ng	576896	Phenanthrene-d10	11.363

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	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			Octadecanoic acid	284	C18H36O2	000057-11-4	64



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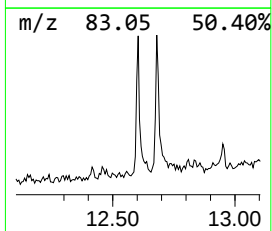
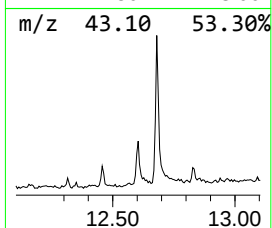
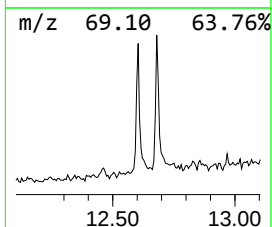
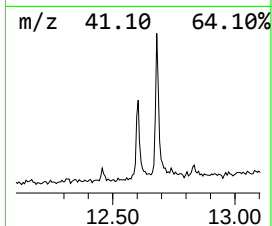
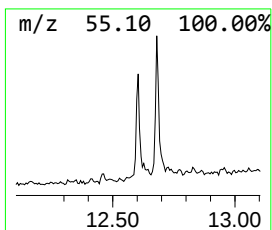
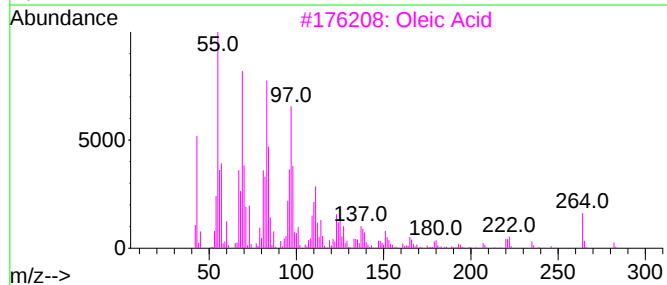
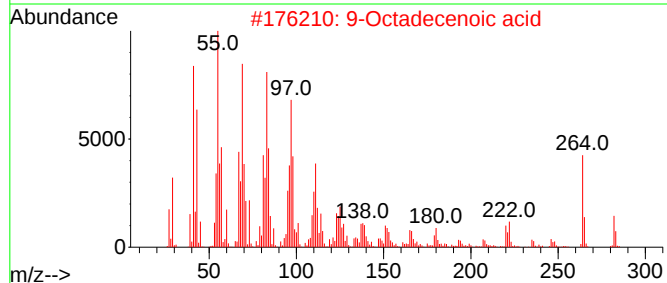
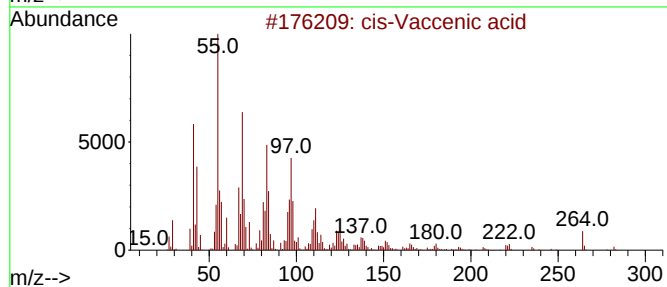
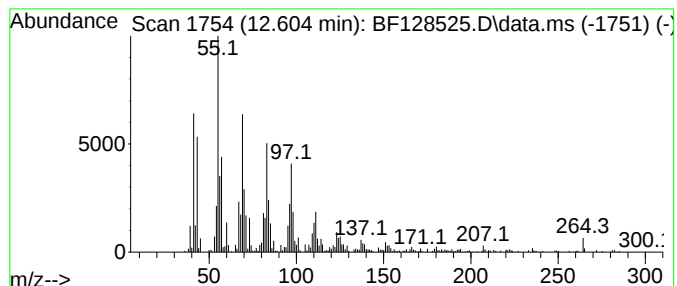
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 cis-Vaccenic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.604	3.49 ng	321855	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-Vaccenic acid	282	C18H34O2	000506-17-2	98
2			9-Octadecenoic acid	282	C18H34O2	002027-47-6	98
3			Oleic Acid	282	C18H34O2	000112-80-1	95
4			6-Octadecenoic acid	282	C18H34O2	1000336-66-8	94
5			Palmitoleic acid	254	C16H30O2	000373-49-9	91



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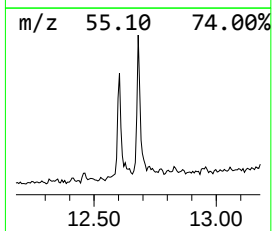
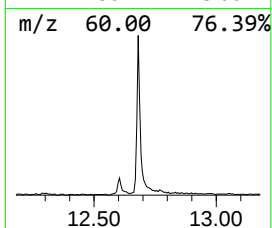
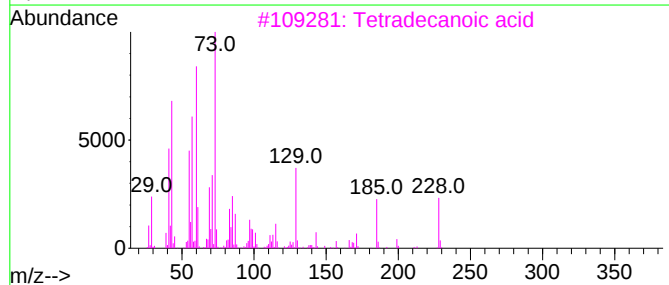
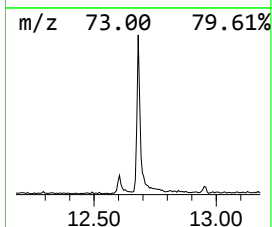
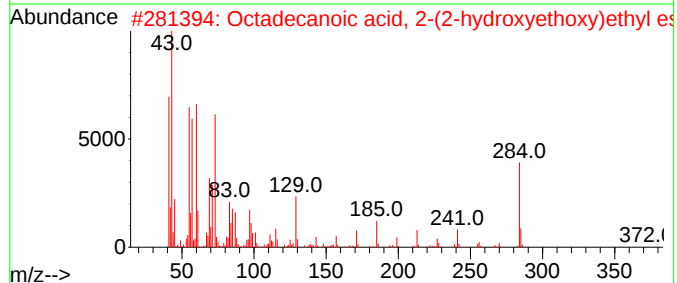
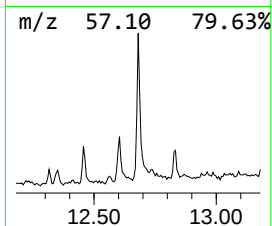
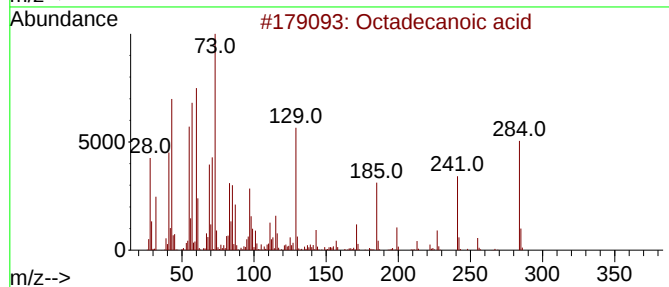
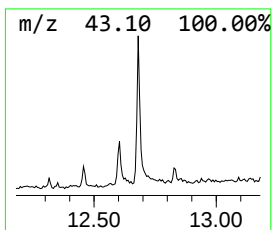
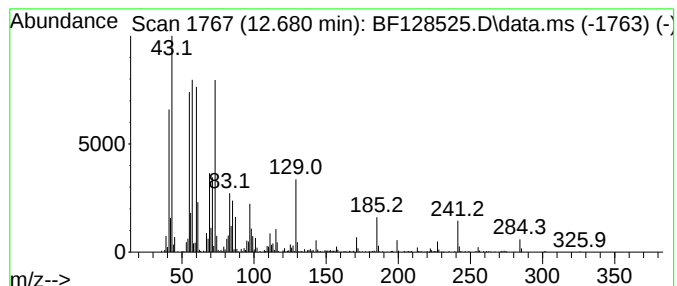
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.680	7.00 ng	645836	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	60
5			n-Decanoic acid	172	C10H20O2	000334-48-5	53



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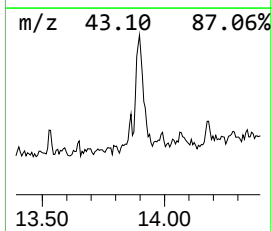
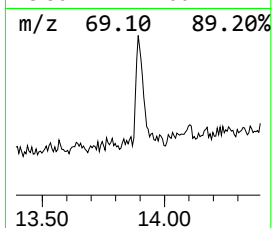
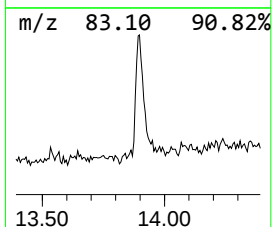
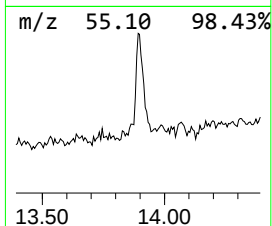
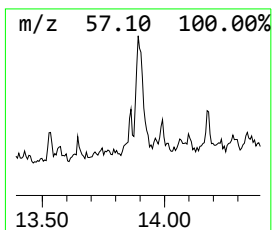
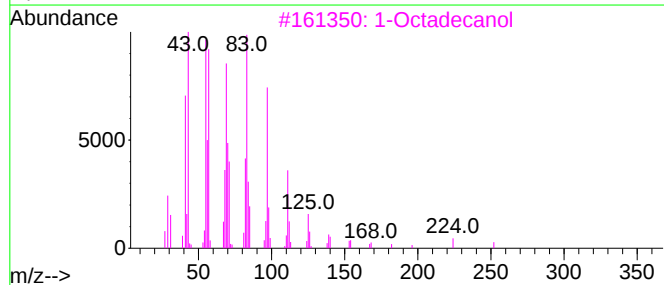
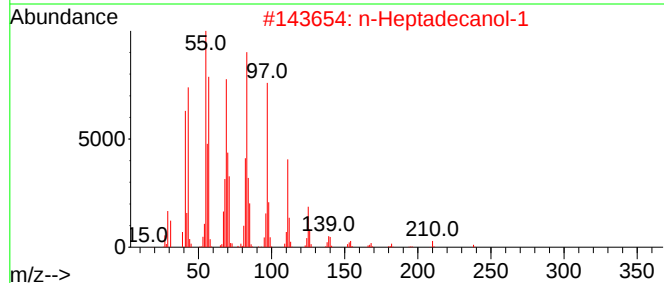
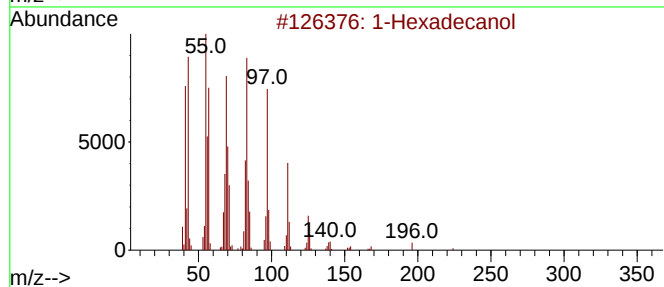
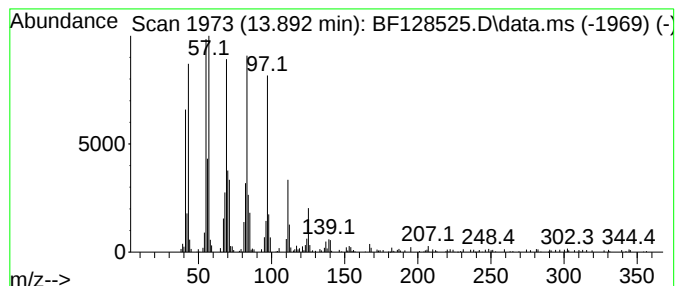
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1-Hexadecanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	6.93 ng	411954	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexadecanol	242	C16H34O	036653-82-4	95
2			n-Heptadecanol-1	256	C17H36O	001454-85-9	94
3			1-Octadecanol	270	C18H38O	000112-92-5	94
4			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5			1-Heneicosanol	312	C21H44O	015594-90-8	93



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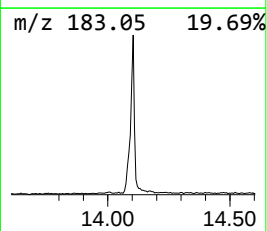
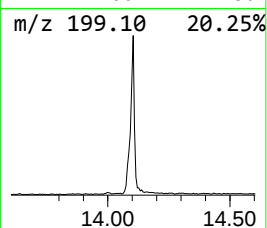
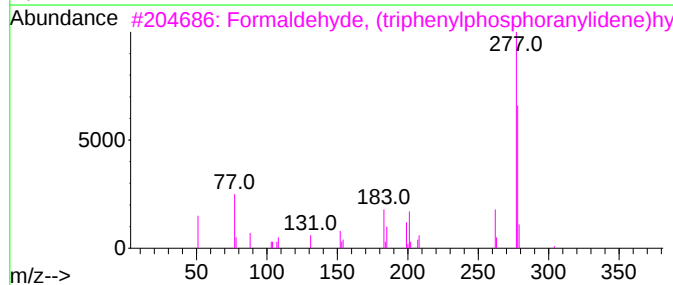
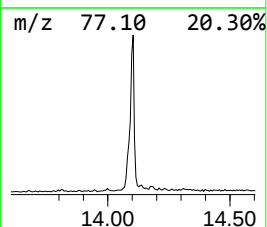
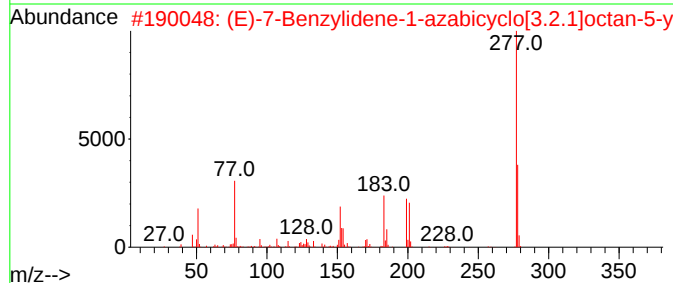
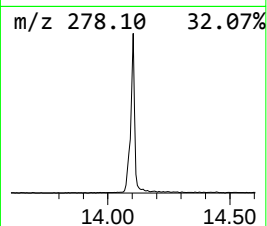
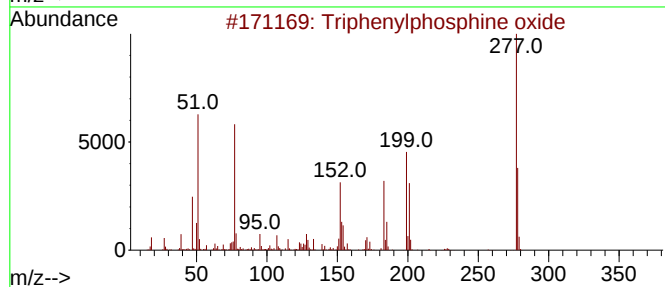
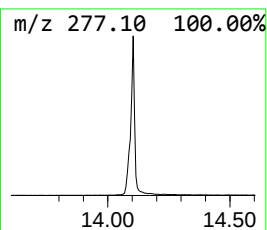
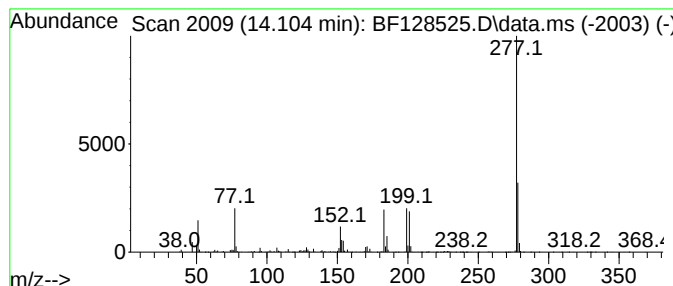
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.104	19.01 ng	1130250	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
4			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	25
5			Thiophene-3-carbonitrile, 4-(4-m...	277	C13H11NO2S2	1000268-75-0	9



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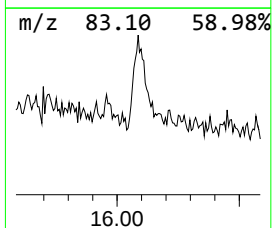
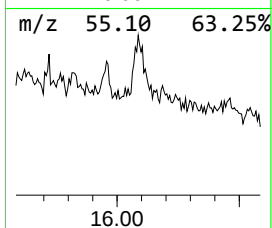
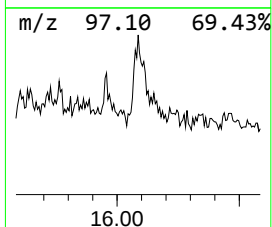
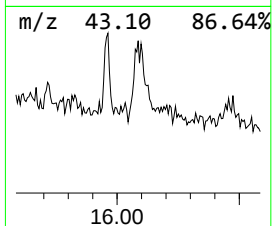
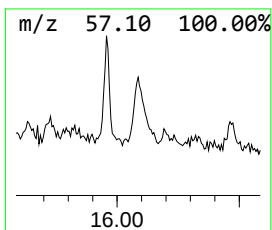
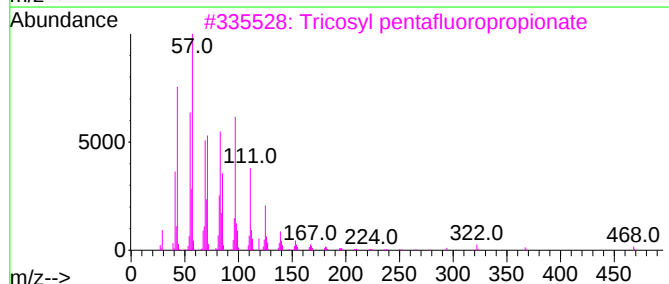
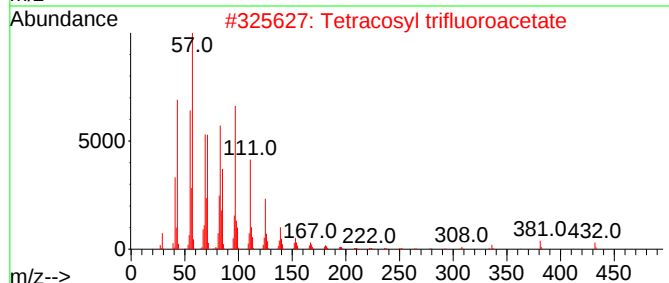
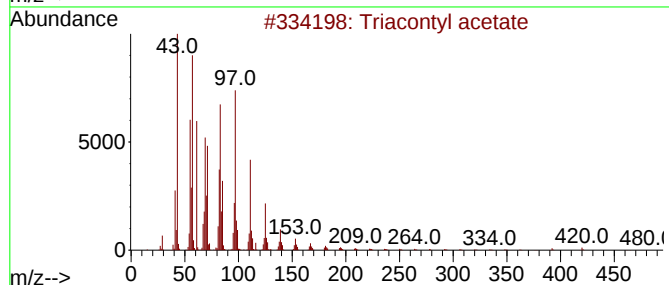
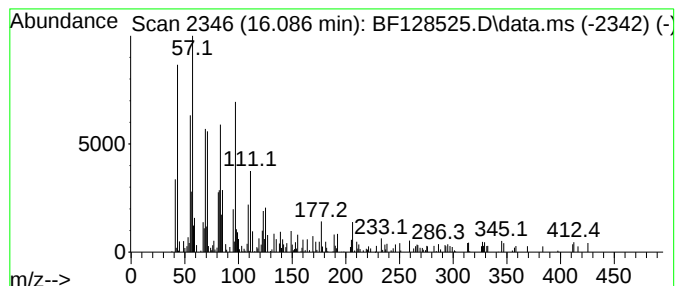
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triacetyl acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.086	2.66 ng	142610	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triacetyl acetate	480	C32H64O2	041755-58-2	60
2			Tetracosyl trifluoroacetate	450	C26H49F3O2	1000351-76-4	60
3			Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	60
4			Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	60
5			Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
Data File : BF128525.D
Acq On : 27 May 2022 23:00
Operator : CG\JU
Sample : N2921-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P013-SS002-0612-01

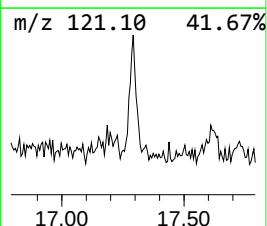
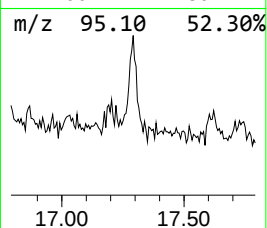
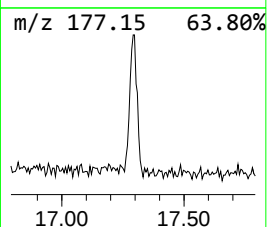
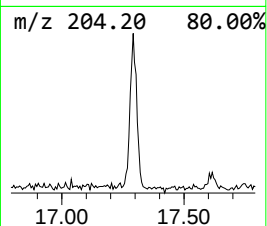
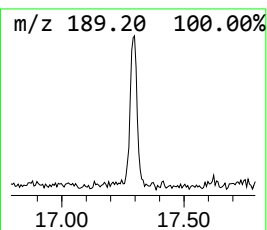
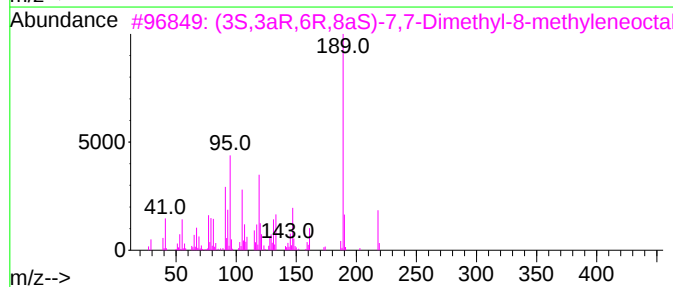
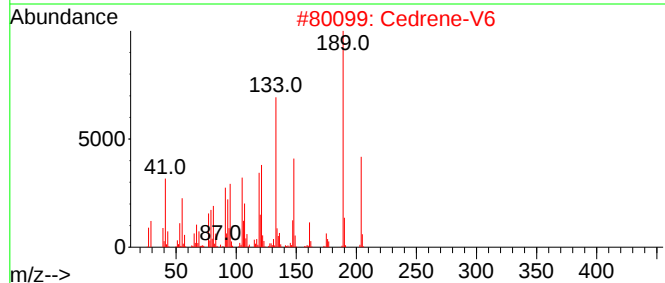
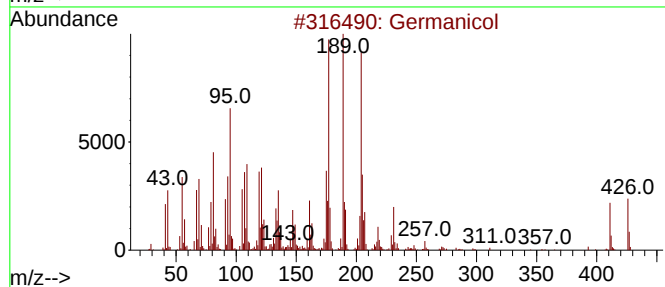
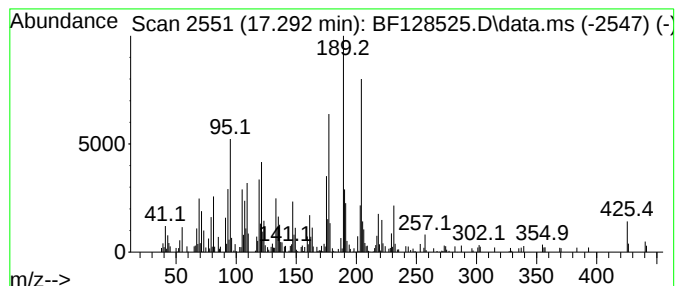
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Germanicol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.292	6.09 ng	326780	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Germanicol	426	C30H50O	000465-02-1	58
2			Cedrene-V6	204	C15H24	1000162-76-8	58
3			(3S,3aR,6R,8aS)-7,7-Dimethyl-8-m...	218	C15H22O	082509-29-3	55
4			4a,8-Dimethyl-2-(prop-1-en-2-yl)...	204	C15H24	103827-22-1	49
5			1,3a-Ethano-3aH-indene, 1,2,3,6,...	204	C15H24	004545-68-0	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
Data File : BF128525.D
Acq On : 27 May 2022 23:00
Operator : CG\JU
Sample : N2921-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P013-SS002-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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
n-Hexadecanoic ...	11.892	6.3	ng	576896	4	11.363	1844540	20.0
cis-Vaccenic acid	12.604	3.5	ng	321855	4	11.363	1844540	20.0
Octadecanoic acid	12.680	7.0	ng	645836	4	11.363	1844540	20.0
1-Hexadecanol	13.892	6.9	ng	411954	5	14.004	1189110	20.0
Triphenylphosph...	14.104	19.0	ng	1130250	5	14.004	1189110	20.0
Triacetyl acetate	16.086	2.7	ng	142610	6	15.468	1073060	20.0
Germanicol	17.292	6.1	ng	326780	6	15.468	1073060	20.0