

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
 Data File : BF128550.D
 Acq On : 28 May 2022 16:06
 Operator : CG\JU
 Sample : N2933-03
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P023-SS001-1824-01

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: BF128550.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.057	467	471	478	rVB	85834	107322	2.77%	0.368%
2	5.451	533	538	541	rBV	3235620	3088664	79.84%	10.581%
3	6.457	704	709	712	rBV	3061833	3197165	82.64%	10.952%
4	6.575	726	729	732	rBV	87680	62128	1.61%	0.213%
5	6.839	770	774	777	rBV	1160288	1046695	27.05%	3.586%
6	7.398	864	869	872	rBV	2415212	2169410	56.07%	7.432%
7	8.116	987	991	995	rBV	1538217	1393681	36.02%	4.774%
8	9.198	1169	1175	1178	rBV	4297207	3868775	100.00%	13.253%
9	9.316	1192	1195	1198	rBV	51133	48737	1.26%	0.167%
10	9.875	1285	1290	1293	rBV	1975871	1602990	41.43%	5.491%
11	10.663	1419	1424	1427	rBV	2636142	2341596	60.53%	8.021%
12	11.363	1539	1543	1546	rBV	1920212	1640986	42.42%	5.621%
13	11.639	1582	1590	1607	rBV8	32993	131357	3.40%	0.450%
14	11.757	1607	1610	1614	rVB	286956	229765	5.94%	0.787%
15	11.886	1629	1632	1637	rBV	66676	61024	1.58%	0.209%
16	12.469	1722	1731	1734	rBV	765206	735036	19.00%	2.518%
17	12.551	1742	1745	1751	rBV	212633	193310	5.00%	0.662%
18	12.616	1752	1756	1759	rBV	157741	140954	3.64%	0.483%
19	12.951	1808	1813	1816	rBV	4064424	3674880	94.99%	12.589%
20	13.904	1969	1975	1987	rBV5	61052	199322	5.15%	0.683%
21	13.998	1987	1991	1995	rBV	1282469	1181898	30.55%	4.049%
22	14.098	2002	2008	2016	rBV	511399	572424	14.80%	1.961%
23	15.133	2180	2184	2188	rVB	58354	64519	1.67%	0.221%
24	15.462	2235	2240	2246	rBV	750539	968729	25.04%	3.319%
25	15.951	2318	2323	2331	rVB	106736	159299	4.12%	0.546%
26	16.745	2454	2458	2466	rVB5	29635	58139	1.50%	0.199%
27	17.056	2505	2511	2517	rBV2	47533	95039	2.46%	0.326%
28	17.286	2545	2550	2561	rVB7	67796	157811	4.08%	0.541%

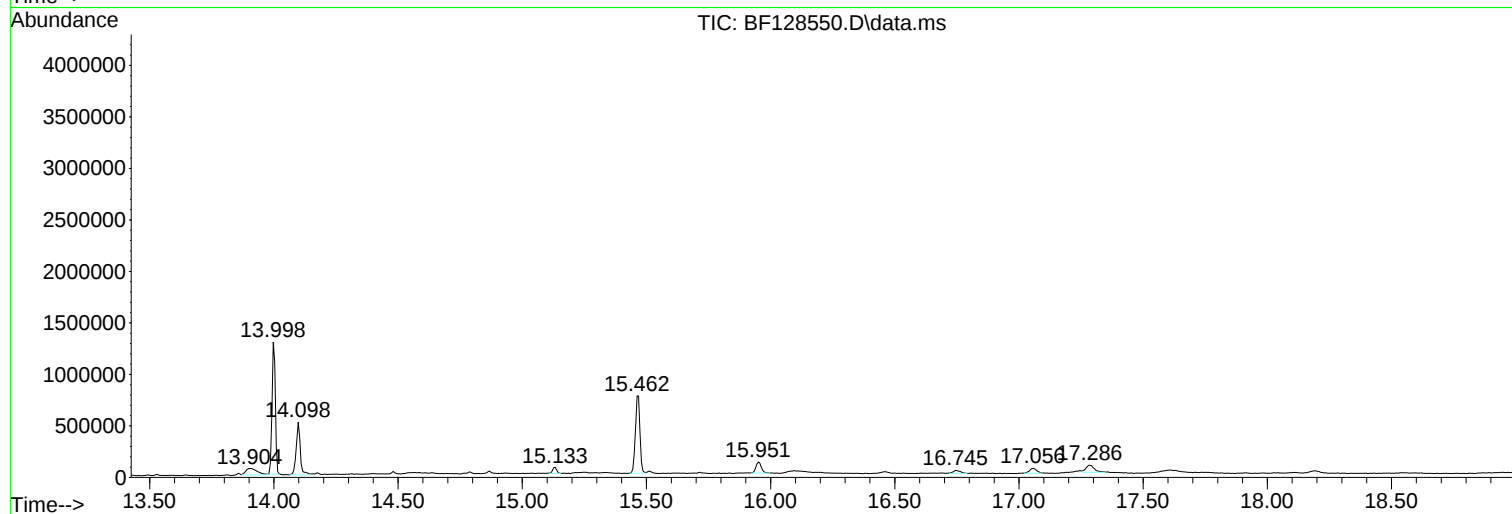
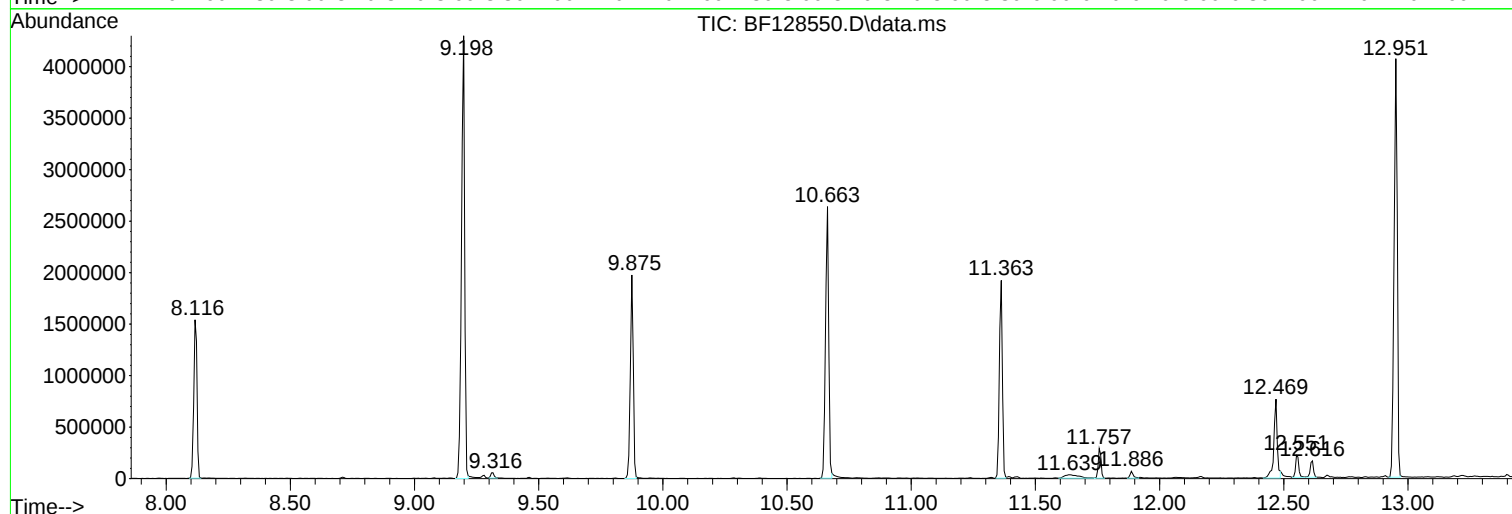
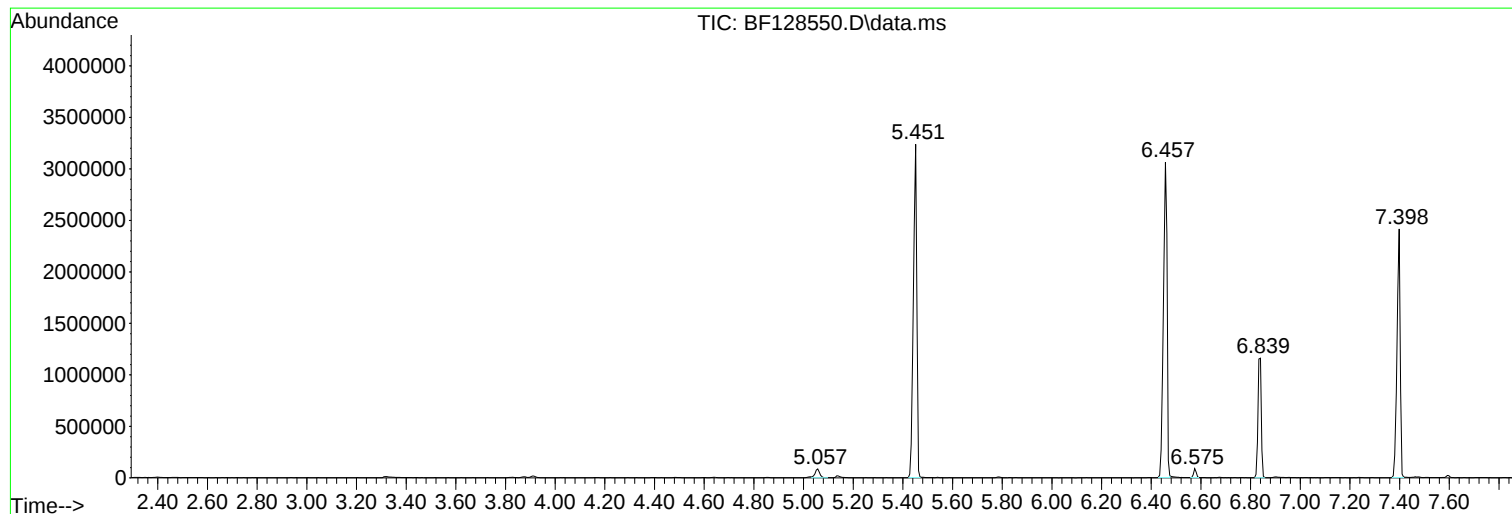
Sum of corrected areas: 29191655

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128550.D
Acq On : 28 May 2022 16:06
Operator : CG\JU
Sample : N2933-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P023-SS001-1824-01

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128550.D
Acq On : 28 May 2022 16:06
Operator : CG\JU
Sample : N2933-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P023-SS001-1824-01

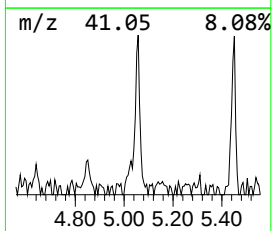
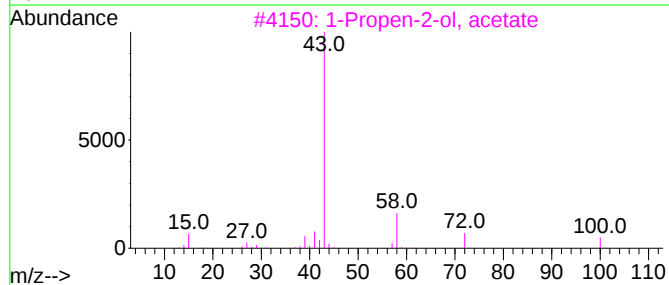
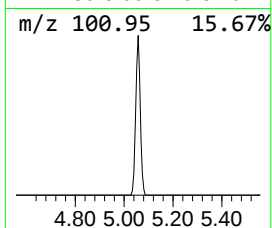
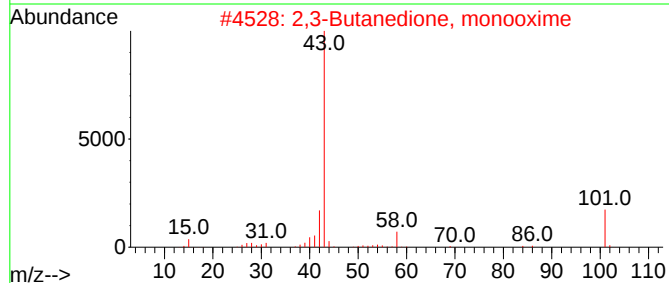
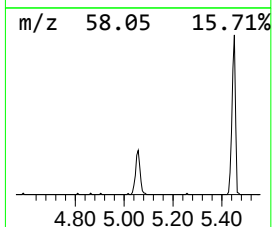
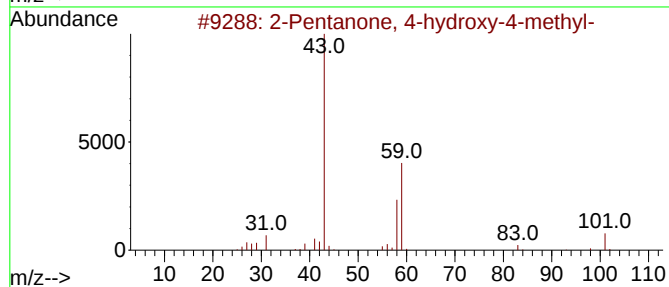
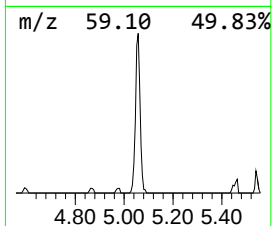
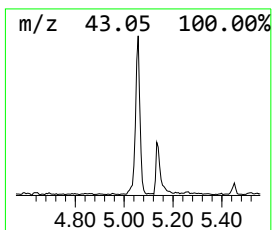
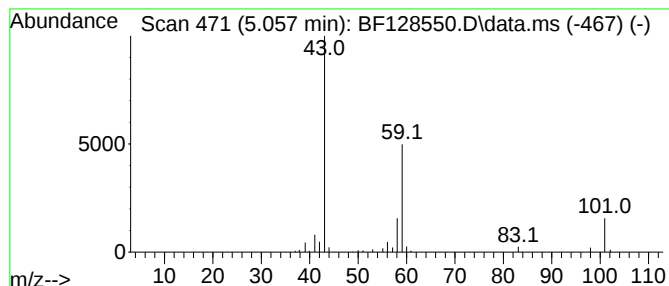
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	2.05 ng	107322	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	Allyl acetate	100	C5H8O2	000591-87-7	9		
5	2-Pentanone, 5-hydroxy-	102	C5H10O2	001071-73-4	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128550.D
Acq On : 28 May 2022 16:06
Operator : CG\JU
Sample : N2933-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

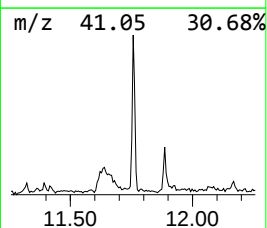
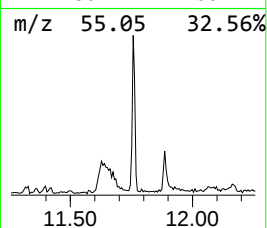
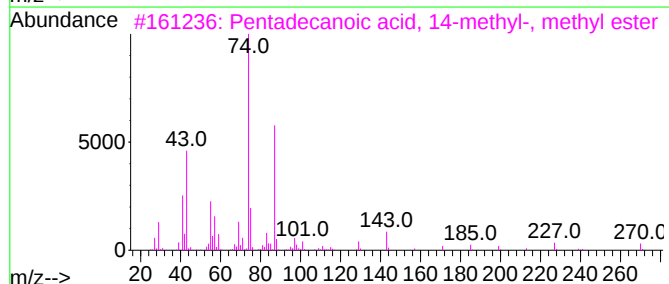
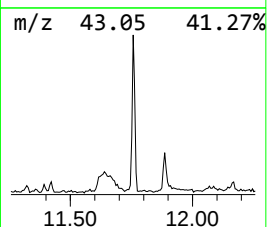
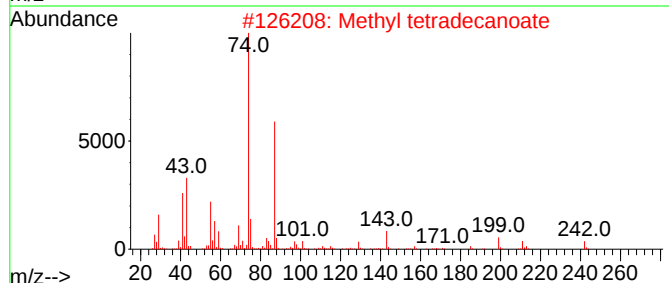
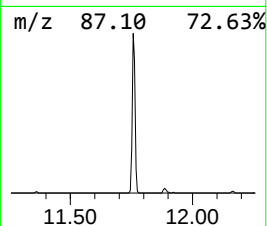
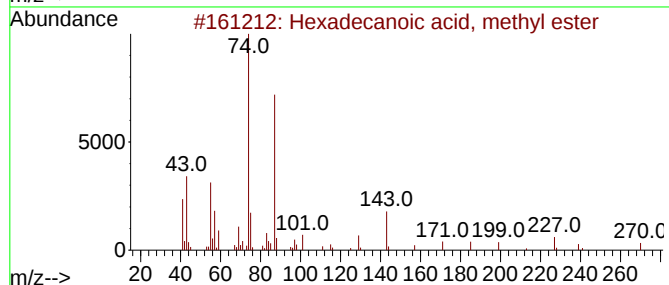
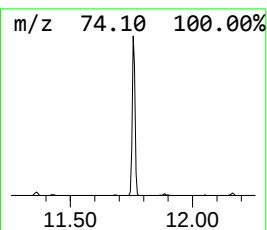
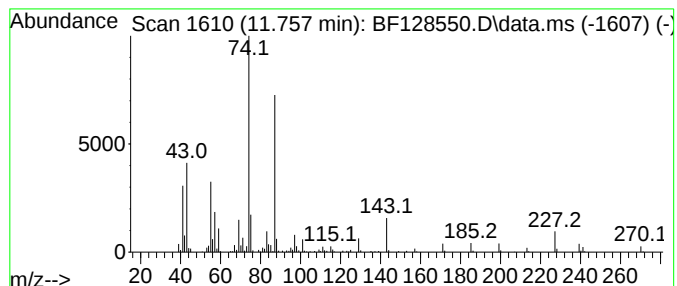
Instrument :
BNA_F
ClientSampleId :
P023-SS001-1824-01

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

Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.757	2.80 ng	229765	Phenanthrene-d10		11.363	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester		270	C17H34O2	000112-39-0	98
2	Methyl tetradecanoate		242	C15H30O2	000124-10-7	91
3	Pentadecanoic acid, 14-methyl-, ...		270	C17H34O2	005129-60-2	87
4	Tridecanoic acid, methyl ester		228	C14H28O2	001731-88-0	87
5	Decanoic acid, methyl ester		186	C11H22O2	000110-42-9	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128550.D
Acq On : 28 May 2022 16:06
Operator : CG\JU
Sample : N2933-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

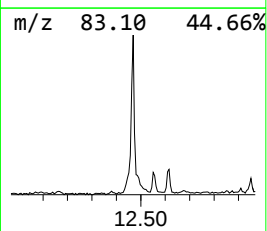
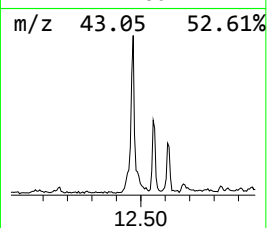
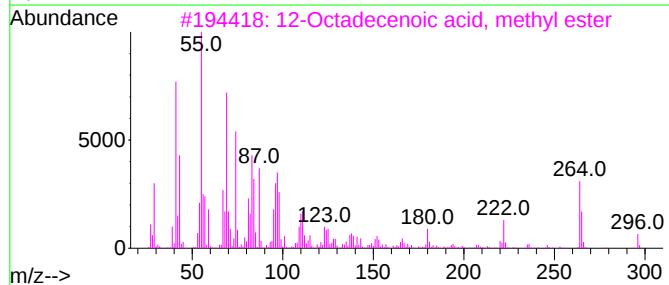
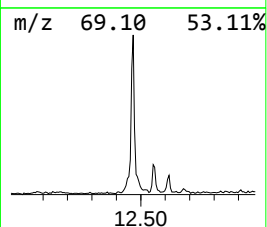
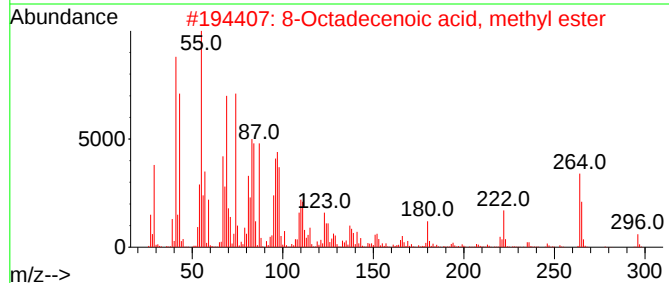
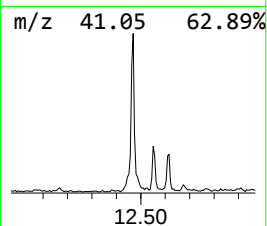
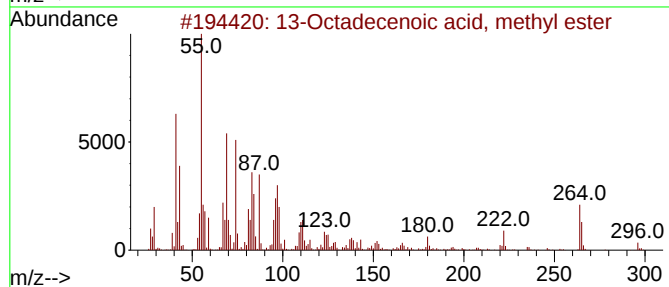
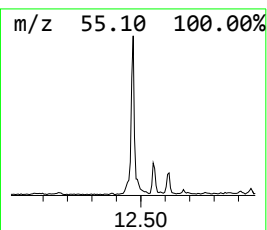
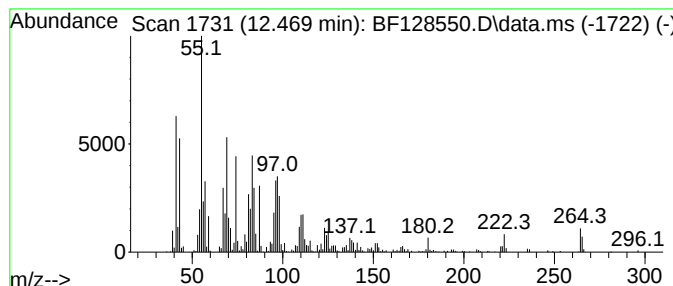
Instrument :
BNA_F
ClientSampleId :
P023-SS001-1824-01

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

Peak Number 3 13-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.469	8.96 ng	735036	Phenanthrene-d10		11.363	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	13-Octadecenoic acid, methyl ester		296	C19H36O2	056554-47-3	99
2	8-Octadecenoic acid, methyl ester		296	C19H36O2	002345-29-1	99
3	12-Octadecenoic acid, methyl ester		296	C19H36O2	056554-46-2	98
4	7-Octadecenoic acid, methyl ester		296	C19H36O2	057396-98-2	97
5	14-Octadecenoic acid, methyl ester		296	C19H36O2	056554-48-4	96



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128550.D
Acq On : 28 May 2022 16:06
Operator : CG\JU
Sample : N2933-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P023-SS001-1824-01

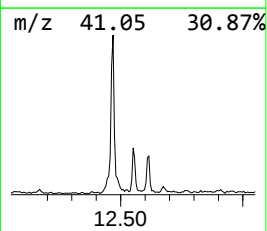
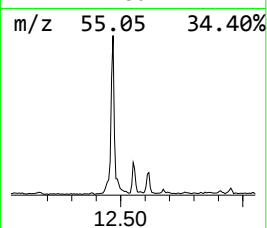
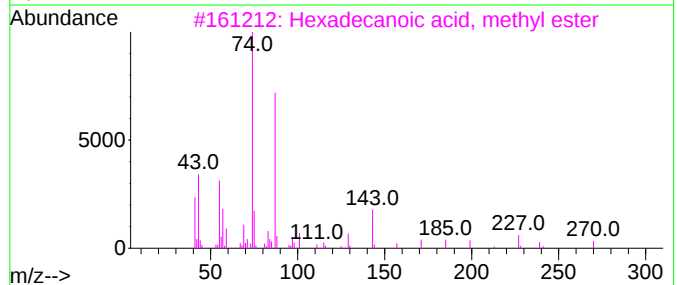
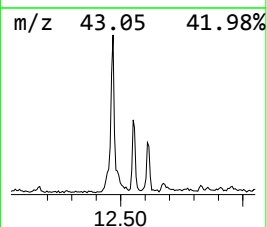
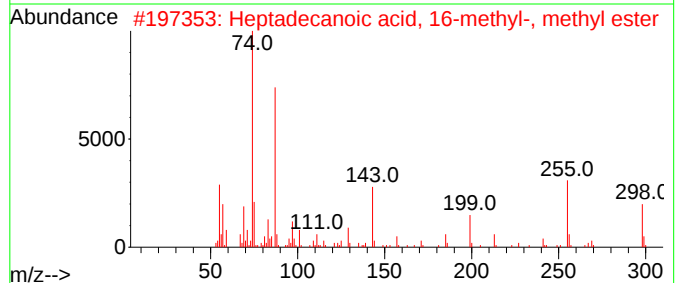
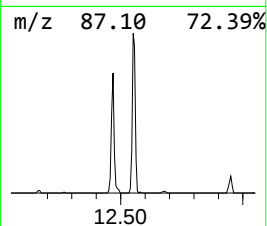
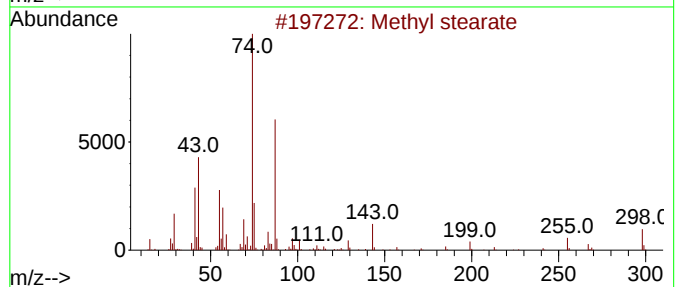
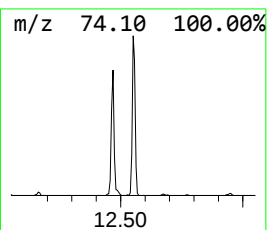
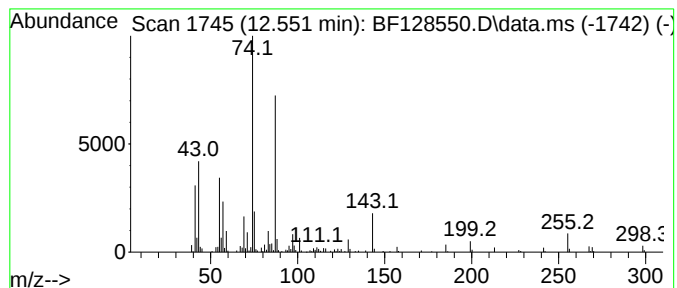
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Methyl stearate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.551	2.36 ng	193310	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	97
2			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	94
3			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	94
4			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	91
5			Methyl tetradecanoate	242	C15H30O2	000124-10-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128550.D
Acq On : 28 May 2022 16:06
Operator : CG\JU
Sample : N2933-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P023-SS001-1824-01

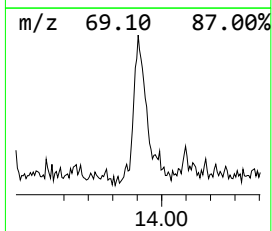
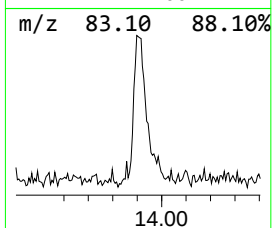
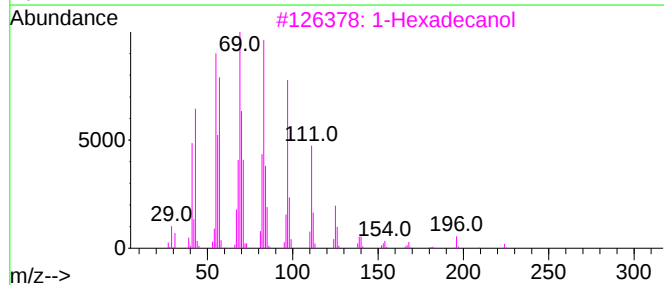
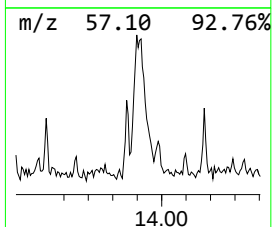
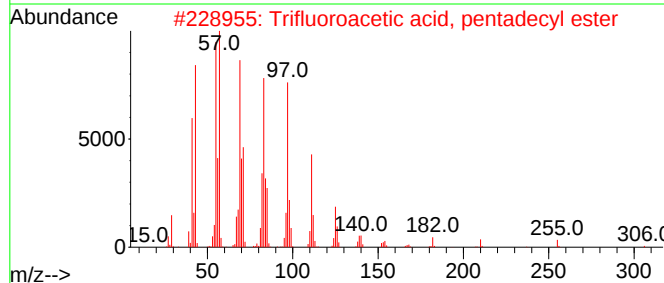
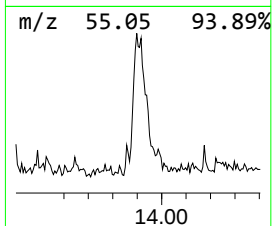
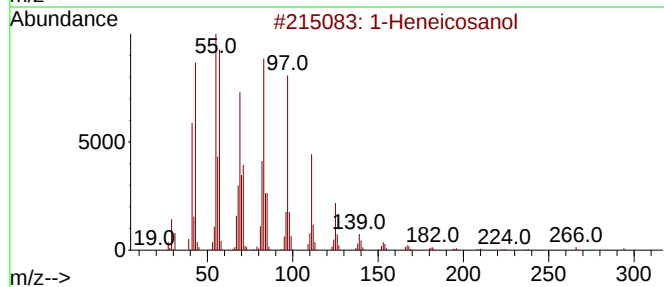
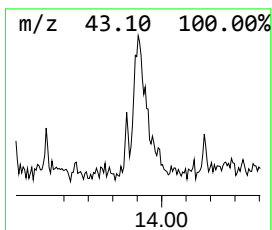
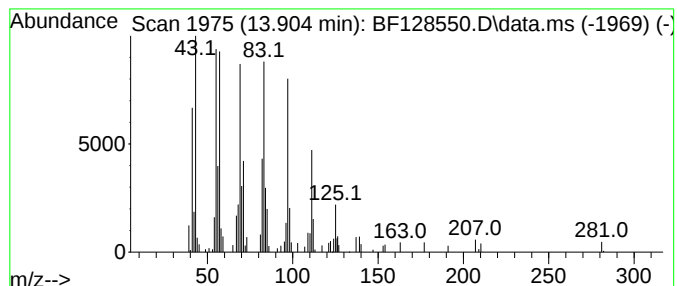
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	3.37 ng	199322	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	93
2			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
3			1-Hexadecanol	242	C16H34O	036653-82-4	91
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
5			1-Pentadecene	210	C15H30	013360-61-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128550.D
Acq On : 28 May 2022 16:06
Operator : CG\JU
Sample : N2933-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P023-SS001-1824-01

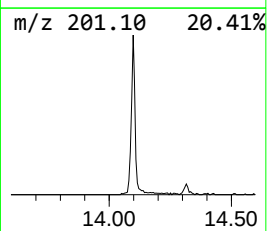
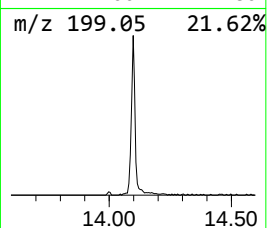
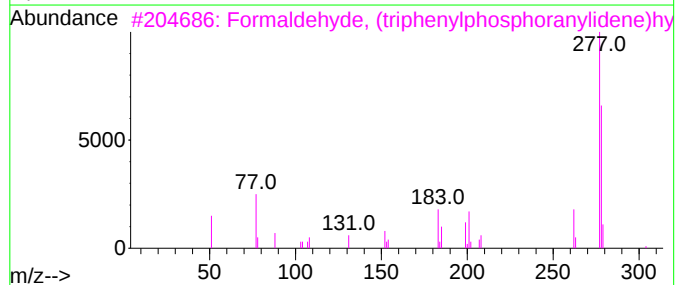
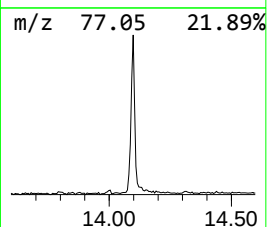
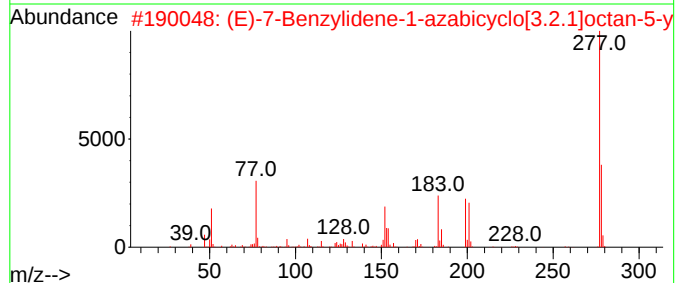
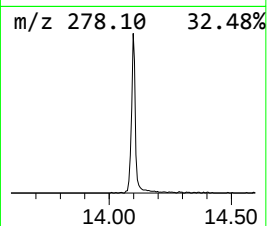
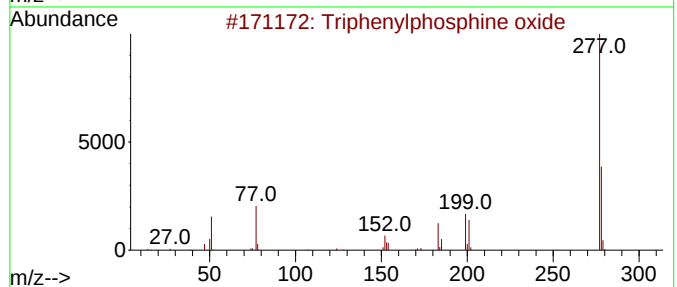
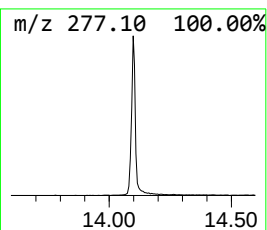
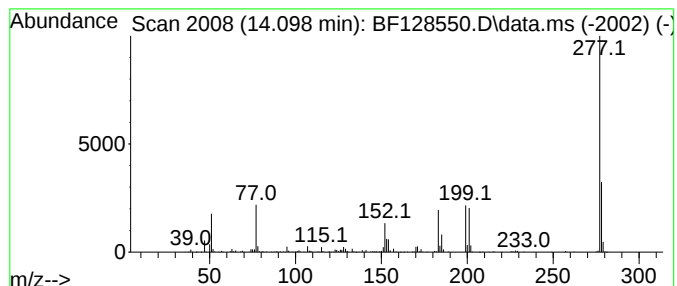
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.098	9.69 ng	572424	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	64
4			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	17
5			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128550.D
Acq On : 28 May 2022 16:06
Operator : CG\JU
Sample : N2933-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P023-SS001-1824-01

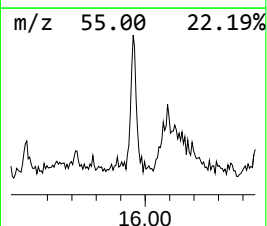
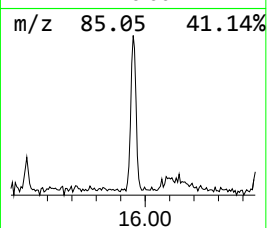
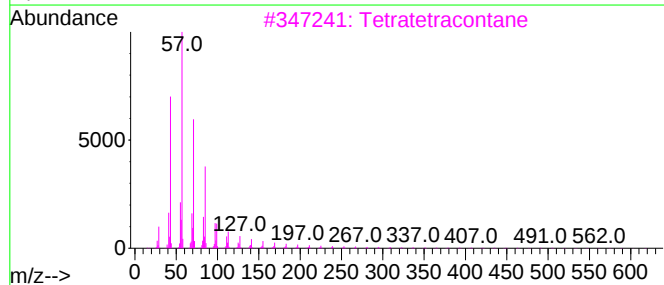
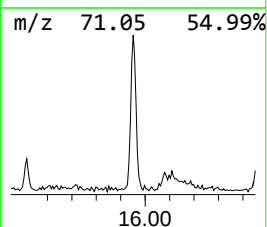
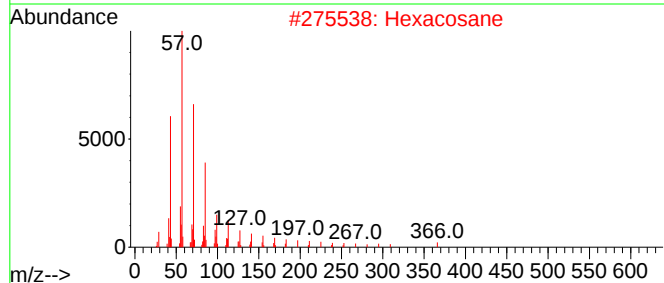
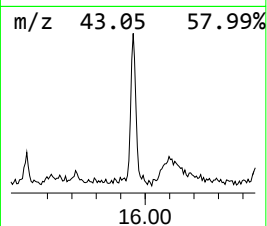
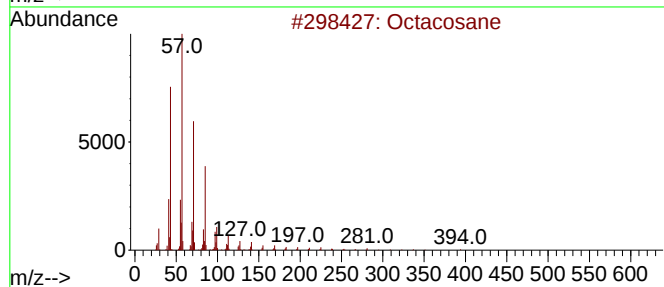
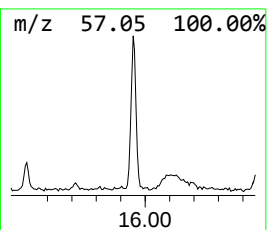
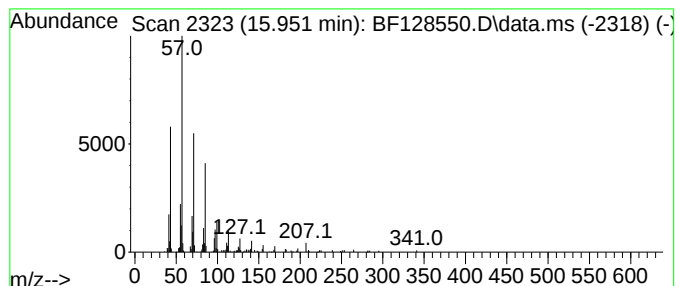
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.951	3.29 ng	159299	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Hexacosane	366	C26H54	000630-01-3	91
3			Tetratetracontane	619	C44H90	007098-22-8	91
4			Hentriacontane	437	C31H64	000630-04-6	91
5			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128550.D
Acq On : 28 May 2022 16:06
Operator : CG\JU
Sample : N2933-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P023-SS001-1824-01

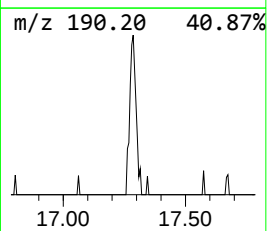
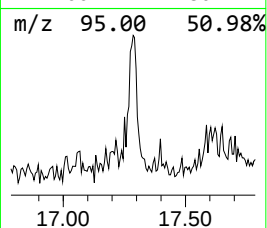
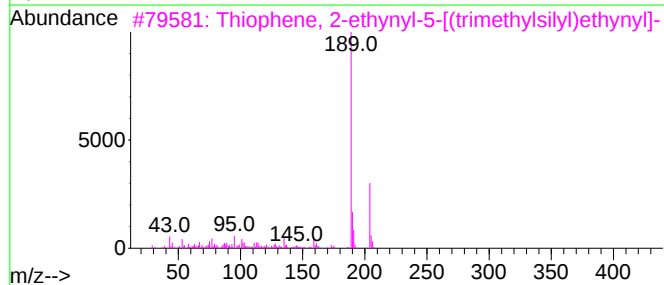
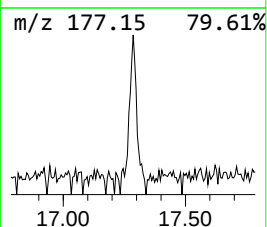
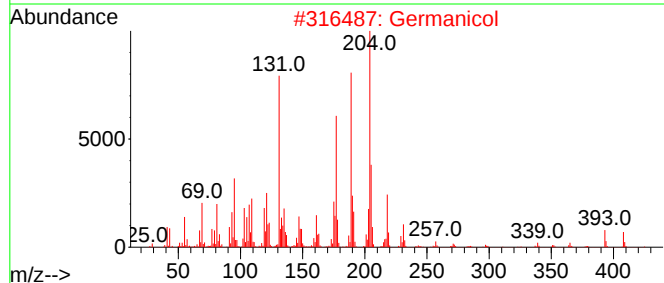
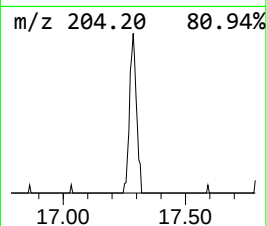
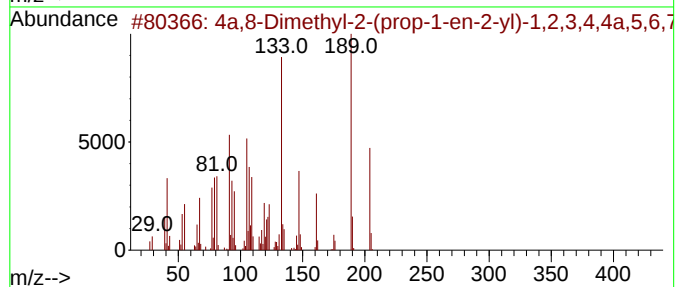
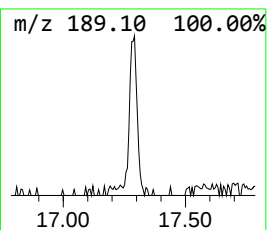
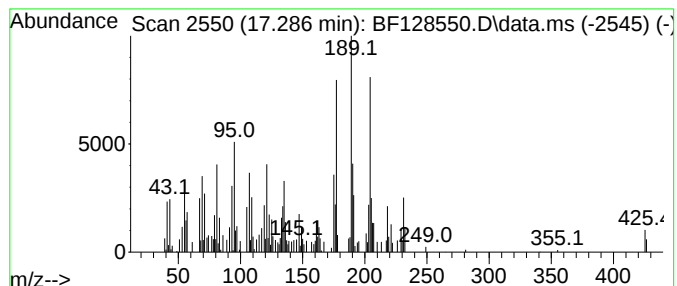
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown17.286 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.286	3.26 ng	157811	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4a,8-Dimethyl-2-(prop-1-en-2-yl)...	204	C15H24	103827-22-1	49		
2	Germanicol	426	C30H50O	000465-02-1	47		
3	Thiophene, 2-ethynyl-5-[(trimeth...	204	C11H12SSi	182323-29-1	46		
4	Hop-22(29)-en-3.beta.-ol	426	C30H50O	058801-23-3	43		
5	trans-.beta.-Ionone	192	C13H20O	000079-77-6	40		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128550.D
Acq On : 28 May 2022 16:06
Operator : CG\JU
Sample : N2933-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P023-SS001-1824-01

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
2-Pentanone, 4-...	5.057	2.0	ng	107322	1	6.839	1046700	20.0
Hexadecanoic ac...	11.757	2.8	ng	229765	4	11.363	1640990	20.0
13-Octadecenoic...	12.469	9.0	ng	735036	4	11.363	1640990	20.0
Methyl stearate	12.551	2.4	ng	193310	4	11.363	1640990	20.0
1-Heneicosanol	13.904	3.4	ng	199322	5	13.998	1181900	20.0
Triphenylphosph...	14.098	9.7	ng	572424	5	13.998	1181900	20.0
Octacosane	15.951	3.3	ng	159299	6	15.468	968729	20.0
unknown17.286	17.286	3.3	ng	157811	6	15.468	968729	20.0