

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042622\
 Data File : BF127929.D
 Acq On : 26 Apr 2022 23:05
 Operator : CG\JU
 Sample : N2551-03
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20220377-096-21-03-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_F\Methods\8270-BF042222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127929.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.863	262	268	275	rBV	35082	48324	1.36%	0.212%
2	5.163	486	489	497	rVB	36395	40314	1.13%	0.177%
3	5.557	552	556	563	rBV	1028680	904882	25.46%	3.968%
4	6.557	722	726	734	rBV	941532	843828	23.74%	3.700%
5	6.675	743	746	749	rBV	47519	40486	1.14%	0.178%
6	6.940	787	791	794	rBV	1094061	911882	25.66%	3.998%
7	7.504	877	887	890	rBV	2194465	2066938	58.16%	9.063%
8	7.610	901	905	912	rVB	53737	57912	1.63%	0.254%
9	7.669	912	915	919	rVB	133656	116409	3.28%	0.510%
10	8.222	1005	1009	1013	rBV	1368955	1190048	33.49%	5.218%
11	8.798	1101	1107	1112	rBV	102607	106165	2.99%	0.465%
12	9.298	1187	1192	1195	rBV	3985965	3553834	100.00%	15.582%
13	9.369	1200	1204	1207	rVB	151877	136029	3.83%	0.596%
14	9.981	1302	1308	1312	rBV	1655740	1415205	39.82%	6.205%
15	10.769	1438	1442	1449	rBV	1581297	1567835	44.12%	6.874%
16	10.822	1449	1451	1457	rVB2	59919	67564	1.90%	0.296%
17	11.475	1558	1562	1565	rBV	1623625	1364849	38.40%	5.984%
18	11.633	1585	1589	1592	rBV	3649645	3158306	88.87%	13.848%
19	11.986	1646	1649	1654	rBV	198426	186810	5.26%	0.819%
20	12.239	1689	1692	1695	rBV	52015	39739	1.12%	0.174%
21	13.057	1827	1831	1835	rBV	2150793	2040925	57.43%	8.949%
22	13.951	1979	1983	1986	rBV2	38660	44322	1.25%	0.194%
23	14.027	1989	1996	2008	rBV3	253433	876186	24.65%	3.842%
24	14.121	2008	2012	2021	rVB	846230	832047	23.41%	3.648%
25	14.880	2138	2141	2148	rVB4	46472	73410	2.07%	0.322%
26	14.974	2153	2157	2161	rVB	173511	179801	5.06%	0.788%
27	15.245	2200	2203	2206	rVB	42722	44147	1.24%	0.194%
28	15.633	2264	2269	2279	rVB	660204	898913	25.29%	3.941%

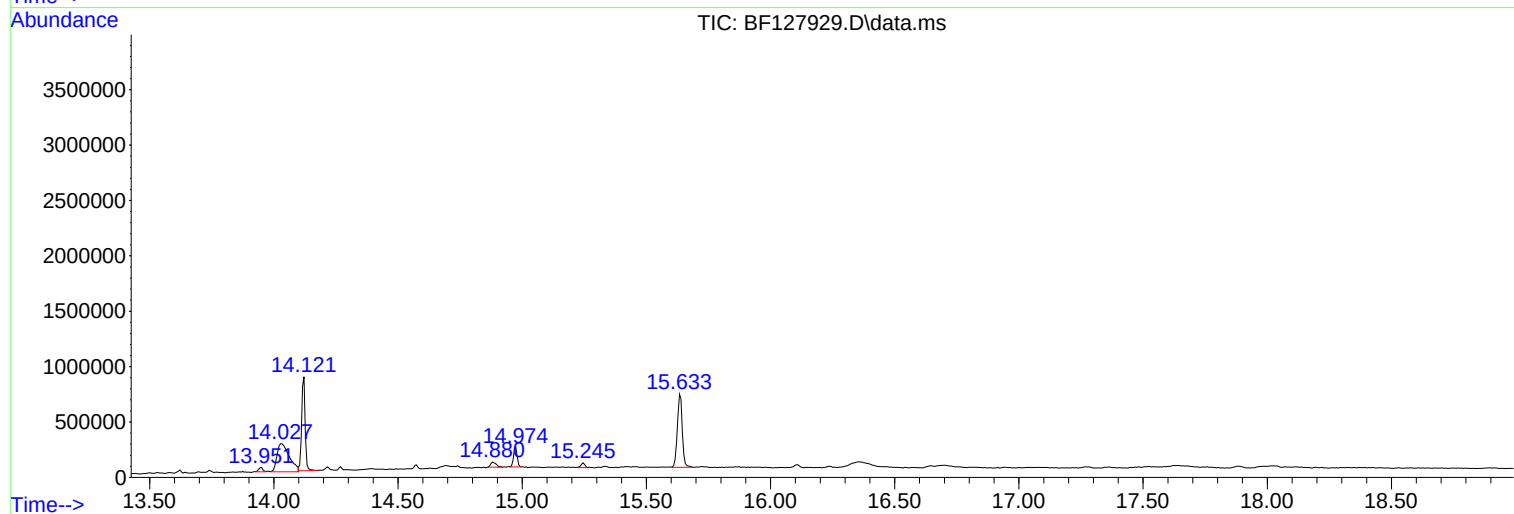
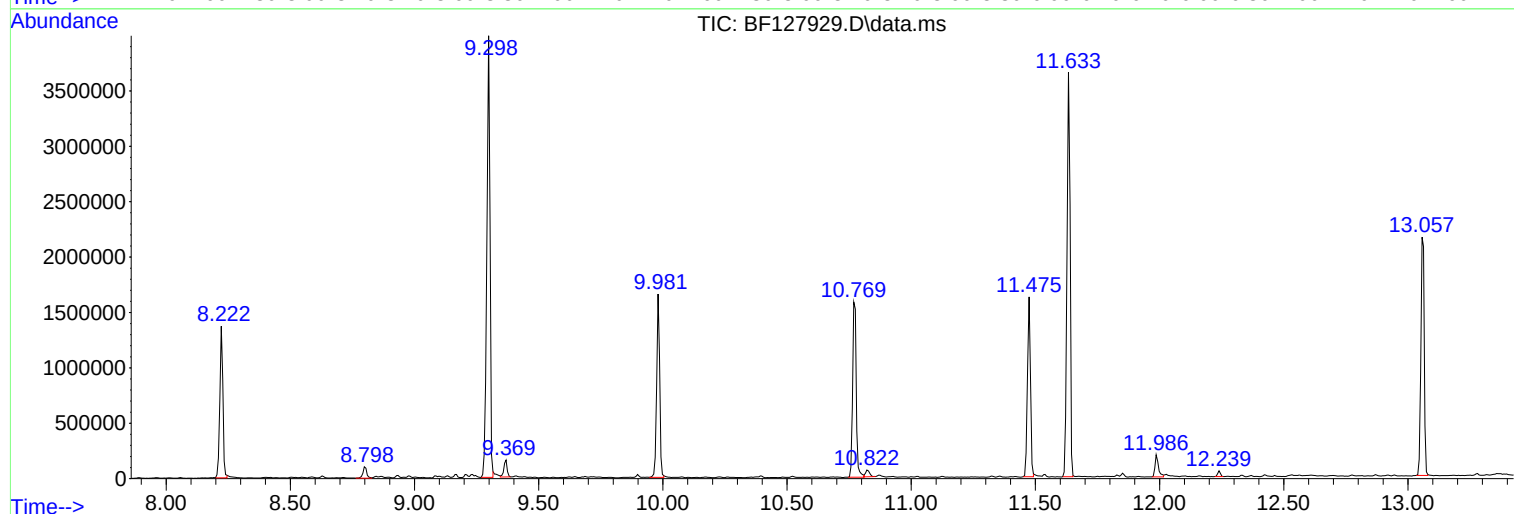
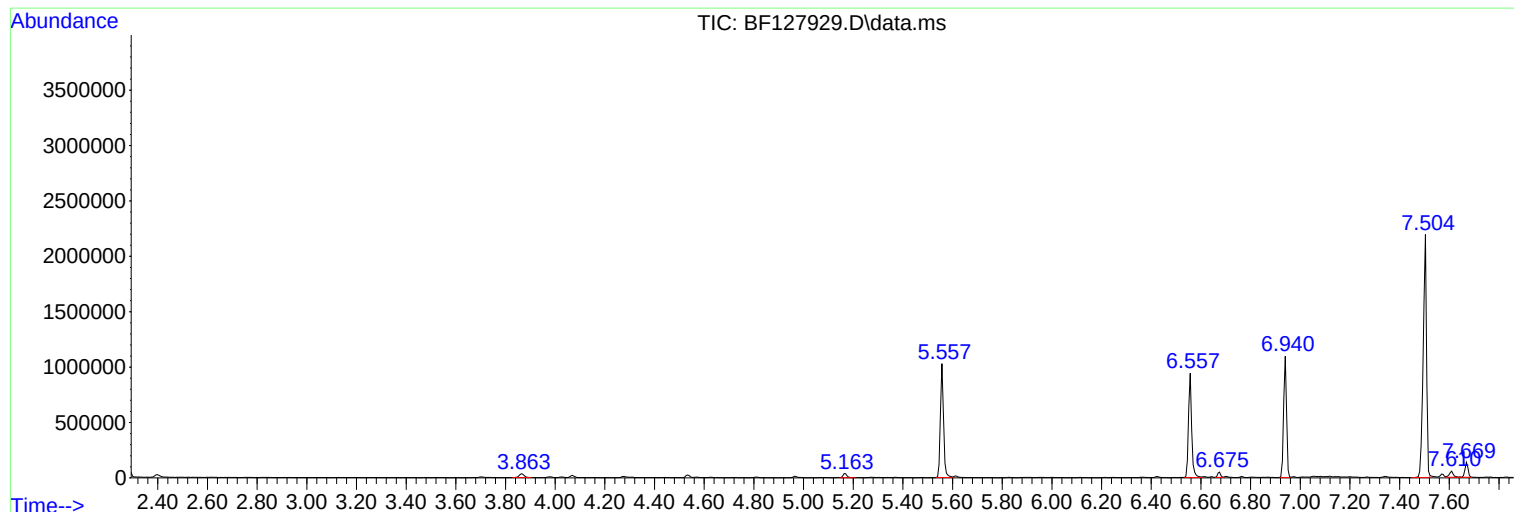
Sum of corrected areas: 22807110

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042622\
Data File : BF127929.D
Acq On : 26 Apr 2022 23:05
Operator : CG\JU
Sample : N2551-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220377-096-21-03-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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\BF042622\
Data File : BF127929.D
Acq On : 26 Apr 2022 23:05
Operator : CG\JU
Sample : N2551-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220377-096-21-03-ELUTRIATE

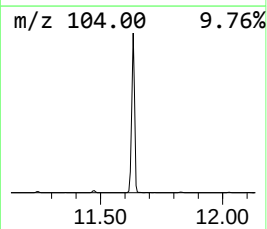
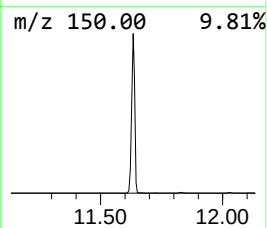
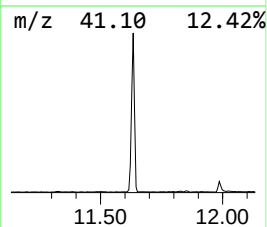
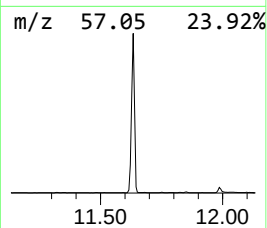
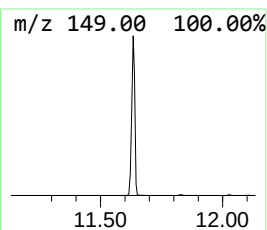
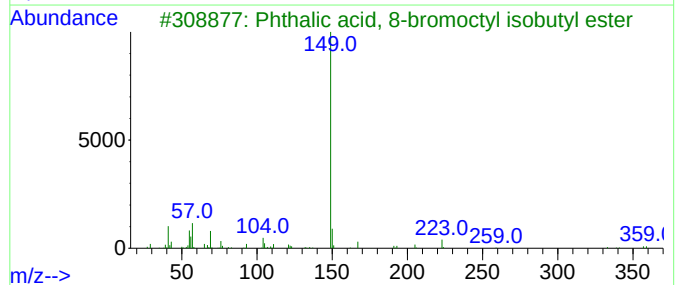
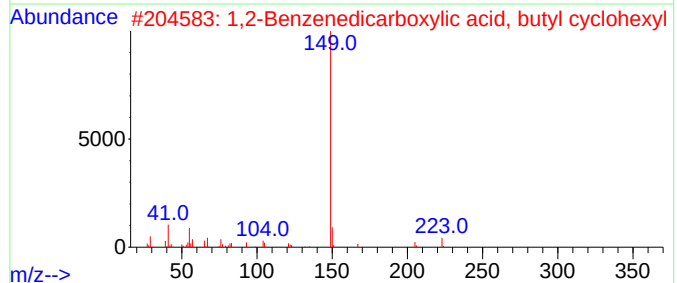
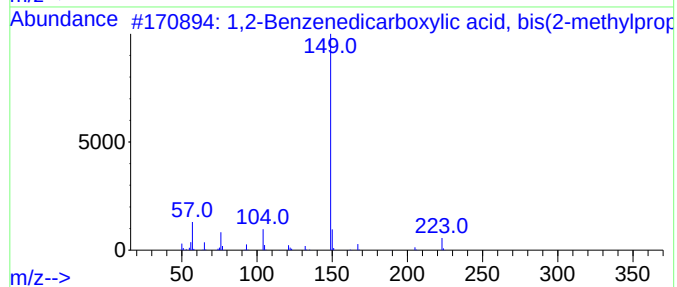
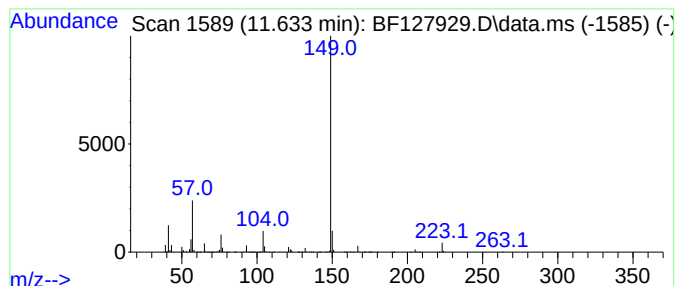
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1,2-Benzenedicarboxylic aci... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.633	46.28 ng	3158310	Phenanthrene-d10	11.475

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	91
2			1,2-Benzenedicarboxylic acid, bu...	304	C18H24O4	000084-64-0	80
3			Phthalic acid, 8-bromooctyl isobu...	412	C20H29BrO4	1000382-55-3	78
4			Phthalic acid, 2-ethoxyethyl pro...	280	C15H20O5	1000322-87-0	78
5			Phthalic acid, hex-2-yn-4-yl iso...	330	C20H26O4	1000315-20-0	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042622\
Data File : BF127929.D
Acq On : 26 Apr 2022 23:05
Operator : CG\JU
Sample : N2551-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220377-096-21-03-ELUTRIATE

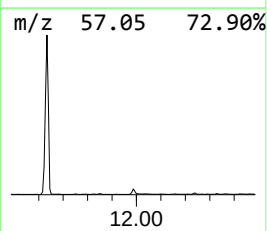
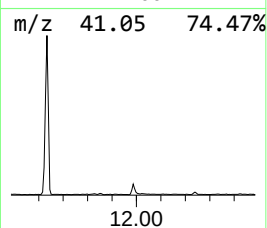
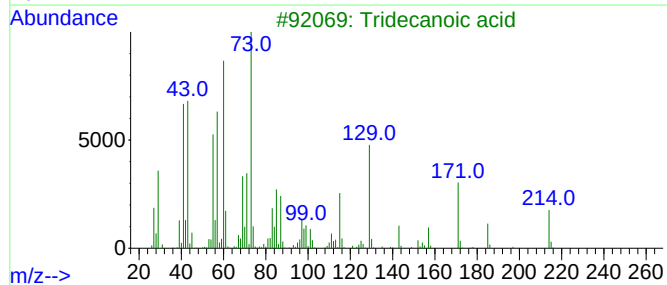
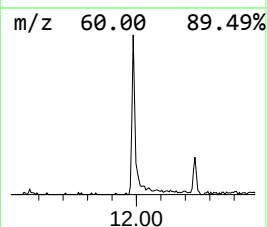
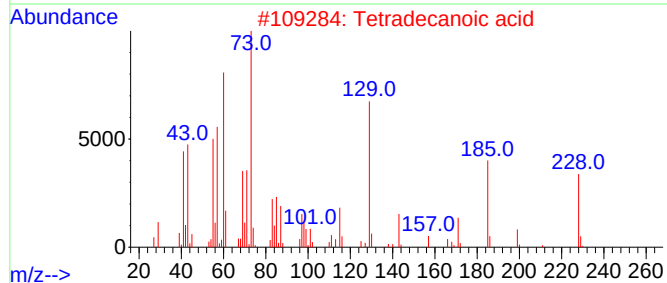
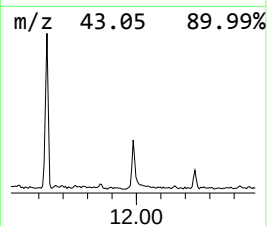
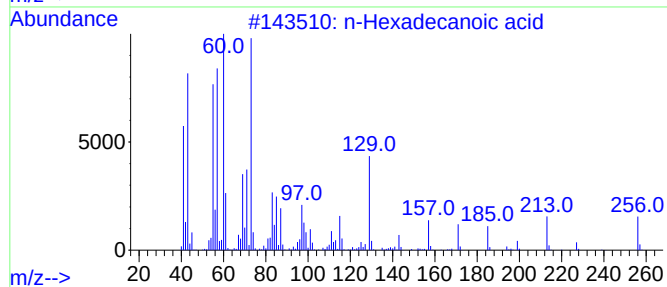
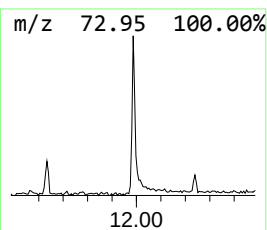
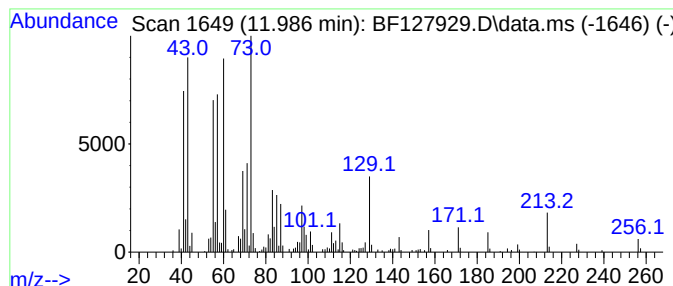
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.986	2.74 ng	186810	Phenanthrene-d10	11.475

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5			Dodecanoic acid	200	C12H24O2	000143-07-7	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042622\
Data File : BF127929.D
Acq On : 26 Apr 2022 23:05
Operator : CG\JU
Sample : N2551-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

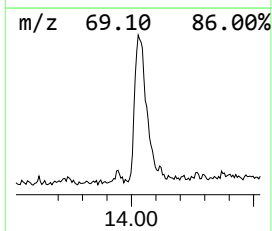
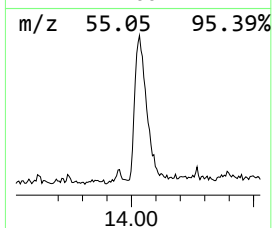
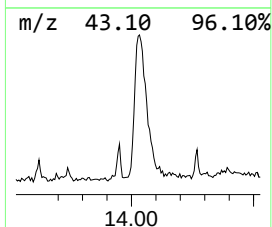
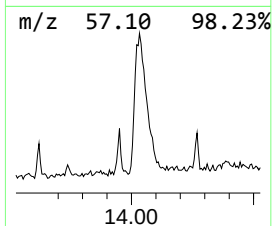
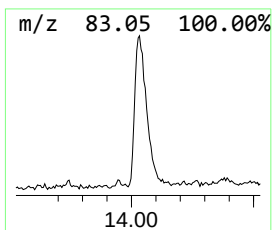
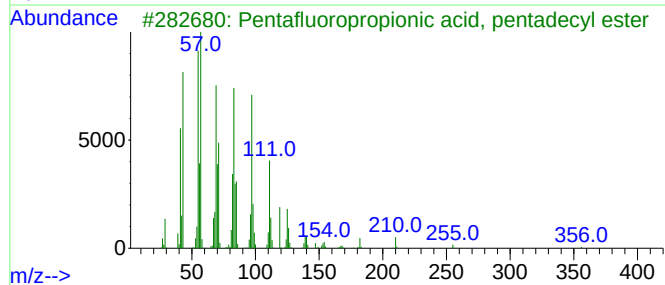
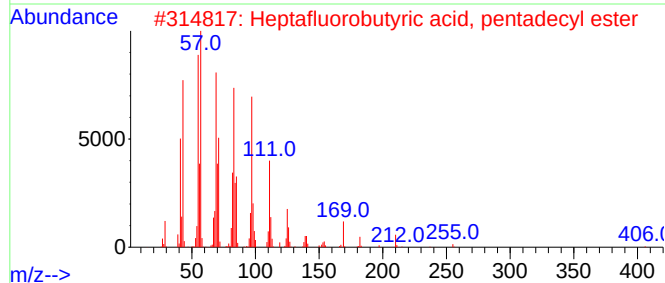
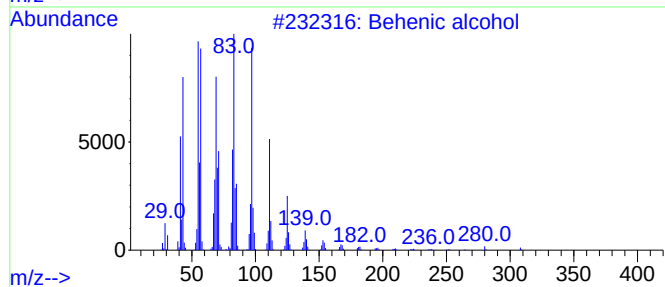
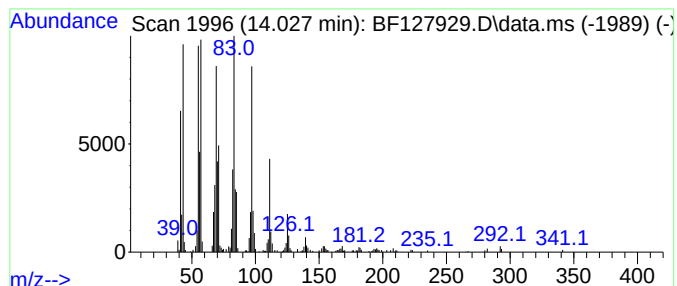
Instrument :
BNA_F
ClientSampleId :
20220377-096-21-03-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Behenic alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.027	21.06 ng	876186	Chrysene-d12		14.121	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Behenic alcohol		326	C22H46O	000661-19-8	94
2	Heptafluorobutyric acid, pentade...		424	C19H31F7O2	959261-23-5	93
3	Pentafluoropropionic acid, penta...		374	C18H31F5O2	959092-08-1	91
4	1-Heneicosanol		312	C21H44O	015594-90-8	91
5	1-Tetracosene		336	C24H48	010192-32-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042622\
Data File : BF127929.D
Acq On : 26 Apr 2022 23:05
Operator : CG\JU
Sample : N2551-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220377-096-21-03-ELUTRIATE

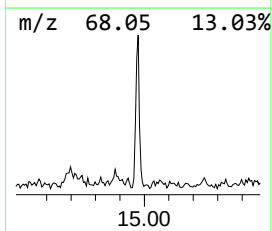
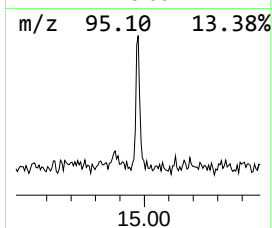
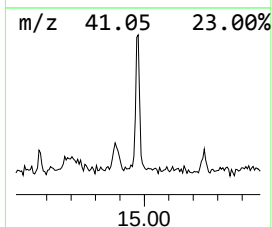
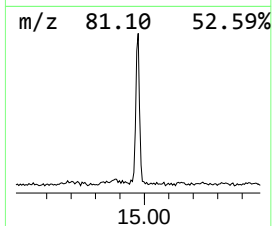
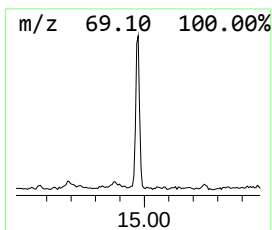
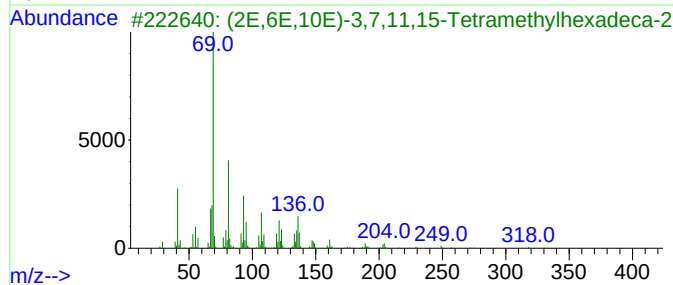
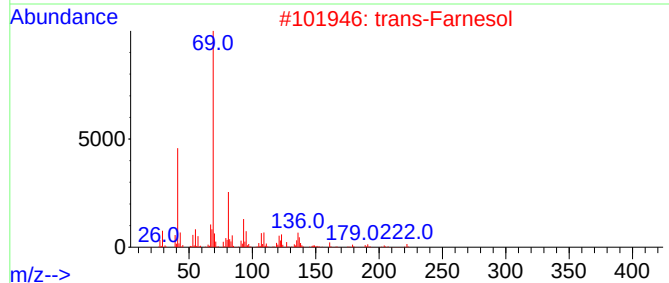
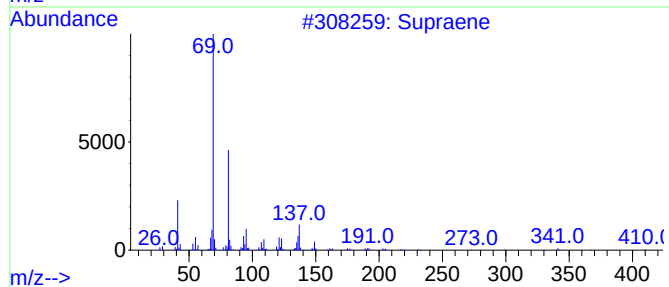
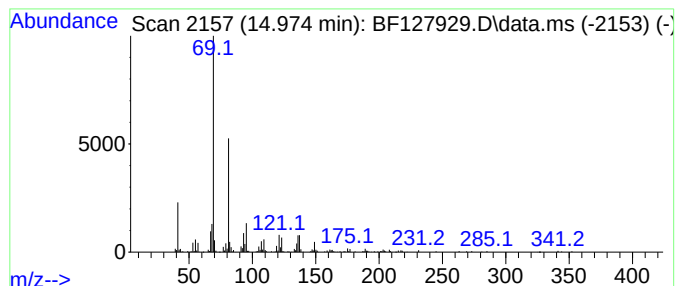
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.974	4.00 ng	179801	Perylene-d12	15.633

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			trans-Farnesol	222	C15H26O	000106-28-5	83
3			(2E,6E,10E)-3,7,11,15-Tetramethy...	318	C21H34O2	125456-63-5	78
4			3-Cyclohexene-1-carboxaldehyde, ...	192	C13H20O	052475-89-5	64
5			(3E,7E)-4,8,12-Trimethyltrideca...	218	C16H26	062235-06-7	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042622\
Data File : BF127929.D
Acq On : 26 Apr 2022 23:05
Operator : CG\JU
Sample : N2551-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220377-096-21-03-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,2-Benzenedica...	11.633	46.3	ng	3158310	4	11.475	1364850	20.0
n-Hexadecanoic ...	11.986	2.7	ng	186810	4	11.475	1364850	20.0
Behenic alcohol	14.027	21.1	ng	876186	5	14.121	832047	20.0
Supraene	14.974	4.0	ng	179801	6	15.633	898913	20.0