

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060823\
 Data File : BF133635.D
 Acq On : 08 Jun 2023 11:25
 Operator : CG\JU
 Sample : 03016-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB28

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-BF052523.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133635.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.051	500	504	510	rBV	45407	54136	1.69%	0.231%
2	5.446	566	571	575	rBV	2077389	2119948	66.06%	9.056%
3	6.463	738	744	747	rBV	2262664	2337114	72.83%	9.984%
4	6.834	803	807	810	rBV	1210131	946507	29.50%	4.043%
5	7.398	898	903	906	rBV	1765248	1468000	45.75%	6.271%
6	8.116	1022	1025	1029	rBV	1518295	1220877	38.05%	5.216%
7	9.198	1204	1209	1212	rBV	3437893	3078599	95.94%	13.152%
8	9.875	1320	1324	1327	rBV	1669462	1313955	40.95%	5.613%
9	10.586	1442	1445	1449	rBV	394425	350814	10.93%	1.499%
10	10.663	1454	1458	1462	rBV	2362610	2316668	72.19%	9.897%
11	11.363	1573	1577	1580	rBV	1654959	1354992	42.22%	5.789%
12	11.886	1663	1666	1677	rBV	186488	200089	6.24%	0.855%
13	12.574	1777	1783	1787	rBV	230891	191369	5.96%	0.818%
14	12.804	1815	1822	1825	rBV	168354	167748	5.23%	0.717%
15	12.957	1843	1848	1851	rBV	3334848	3208982	100.00%	13.709%
16	13.857	1997	2001	2004	rBV2	43983	51869	1.62%	0.222%
17	13.898	2004	2008	2019	rVV5	68828	221106	6.89%	0.945%
18	14.010	2022	2027	2029	rVV	983238	1007545	31.40%	4.304%
19	14.033	2029	2031	2038	rVB	81214	76570	2.39%	0.327%
20	14.480	2104	2107	2110	rBV	47845	43492	1.36%	0.186%
21	14.639	2130	2134	2138	rVB	520453	434600	13.54%	1.857%
22	14.863	2169	2172	2175	rBV	45799	45288	1.41%	0.193%
23	15.045	2199	2203	2206	rBV	54496	86341	2.69%	0.369%
24	15.127	2213	2217	2224	rVB	90915	106239	3.31%	0.454%
25	15.345	2252	2254	2260	rVB	32573	37151	1.16%	0.159%
26	15.474	2270	2276	2280	rBV	716275	882997	27.52%	3.772%
27	15.945	2352	2356	2362	rVB2	58470	85242	2.66%	0.364%

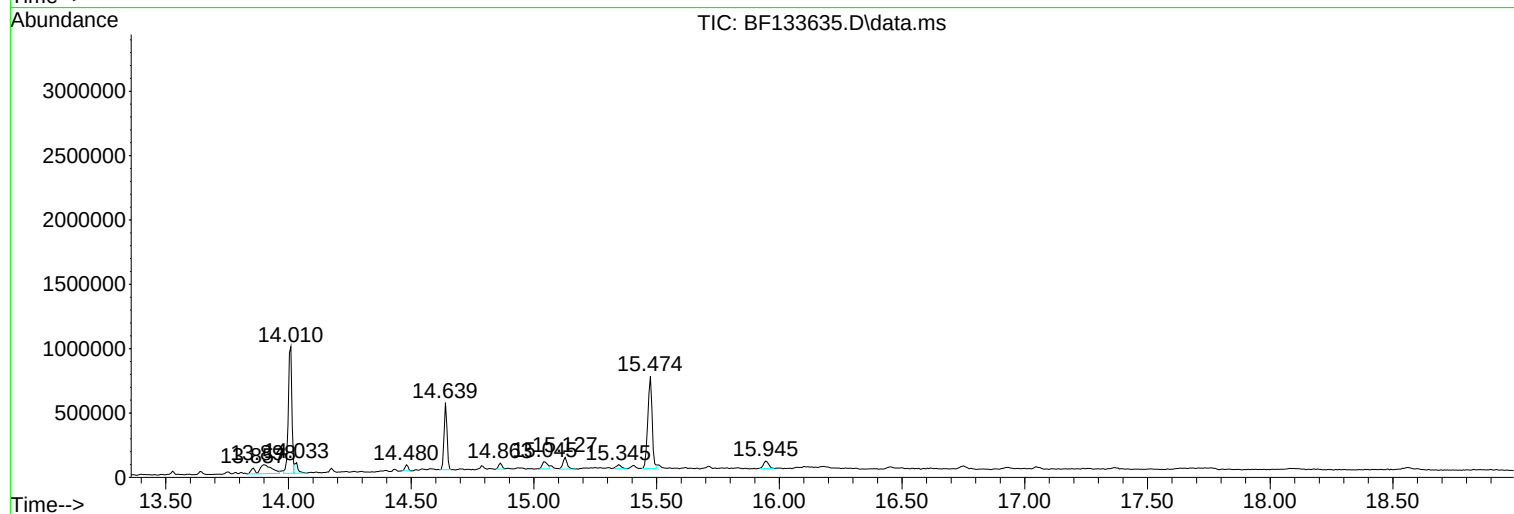
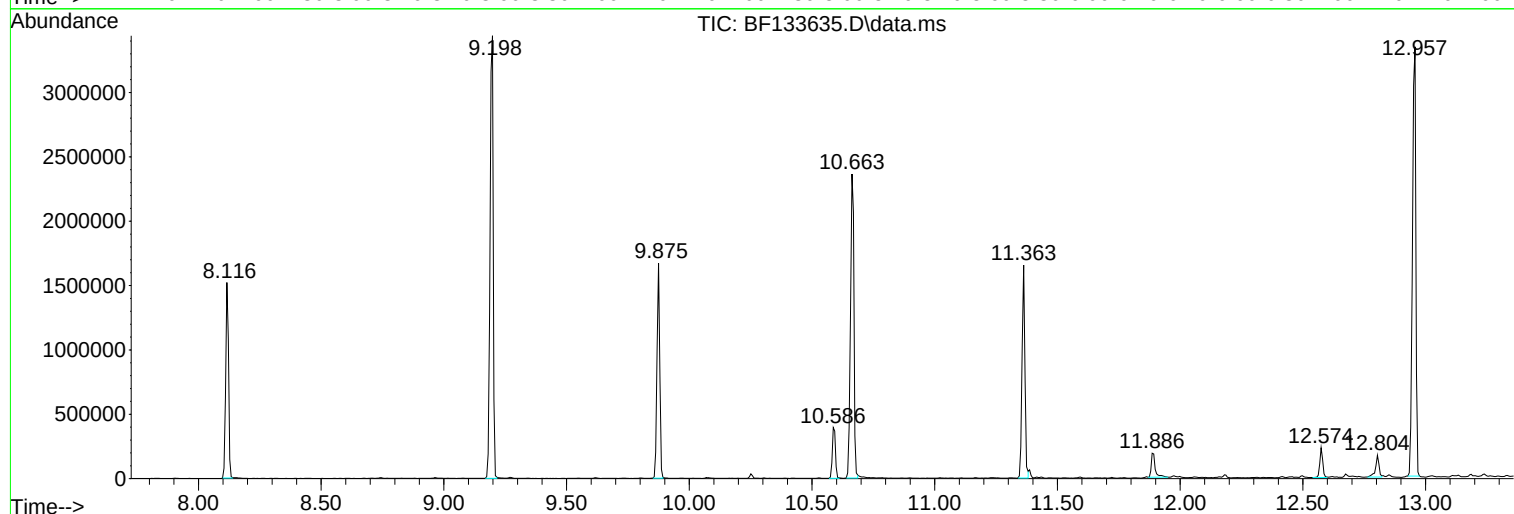
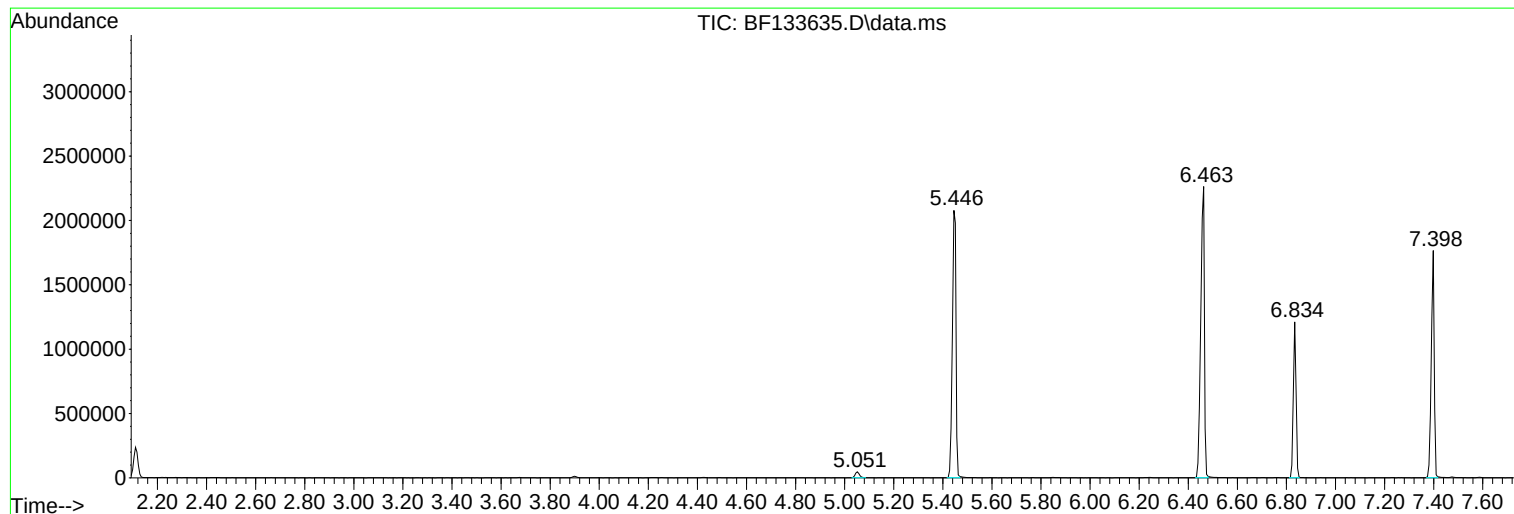
Sum of corrected areas: 23408238

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060823\
Data File : BF133635.D
Acq On : 08 Jun 2023 11:25
Operator : CG\JU
Sample : 03016-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB28

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.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\BF060823\
Data File : BF133635.D
Acq On : 08 Jun 2023 11:25
Operator : CG\JU
Sample : 03016-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB28

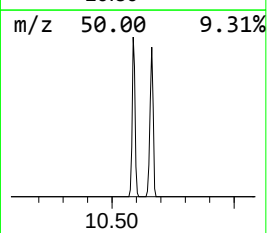
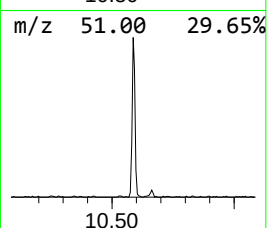
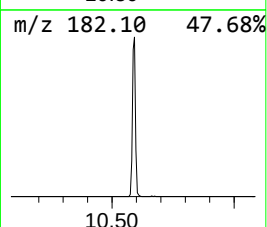
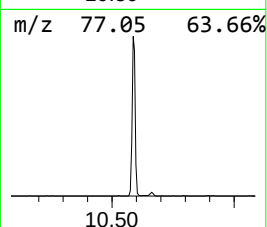
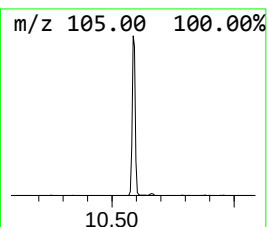
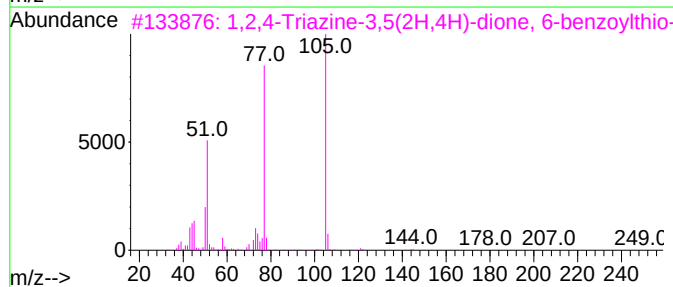
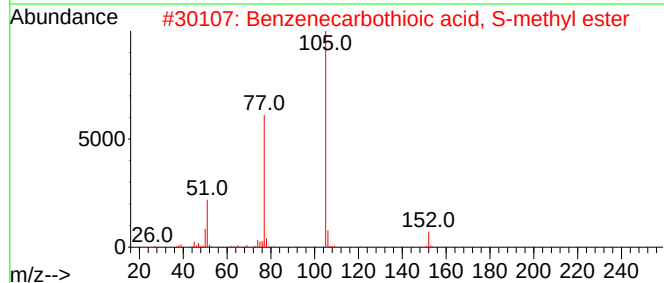
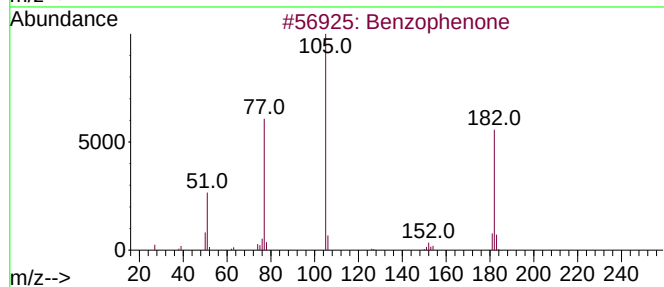
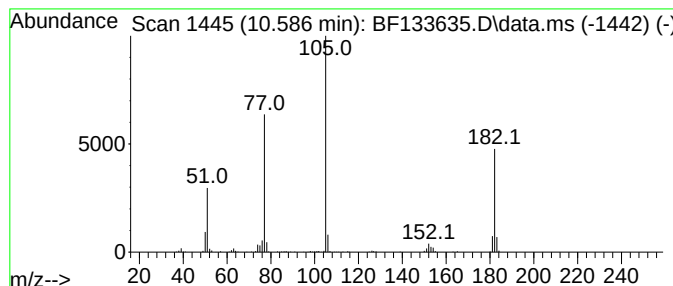
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.586	5.34 ng	350814	Acenaphthene-d10	9.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
3			1,2,4-Triazine-3,5(2H,4H)-dione,...	249	C10H7N3O3S	024168-34-1	50
4			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	50
5			Benzeneacetic acid, .alpha.-oxo-...	178	C10H10O3	001603-79-8	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060823\
Data File : BF133635.D
Acq On : 08 Jun 2023 11:25
Operator : CG\JU
Sample : 03016-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB28

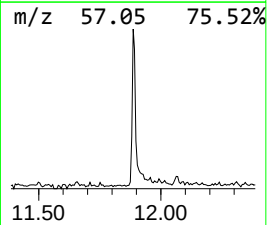
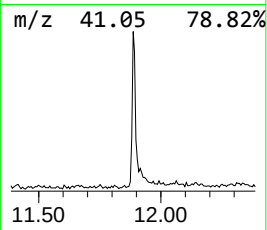
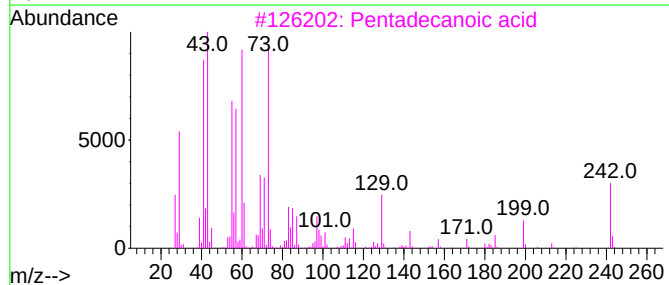
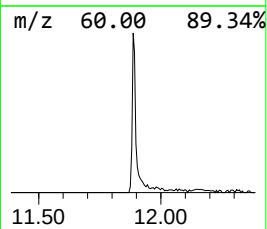
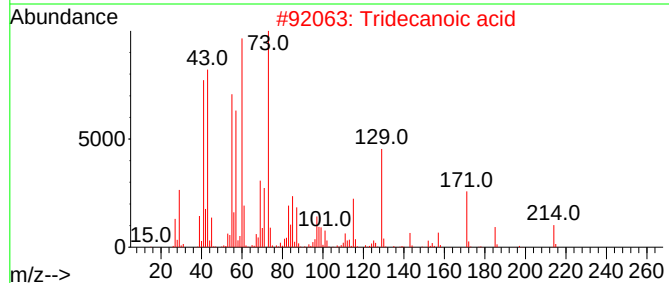
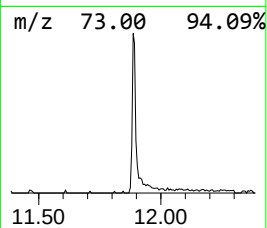
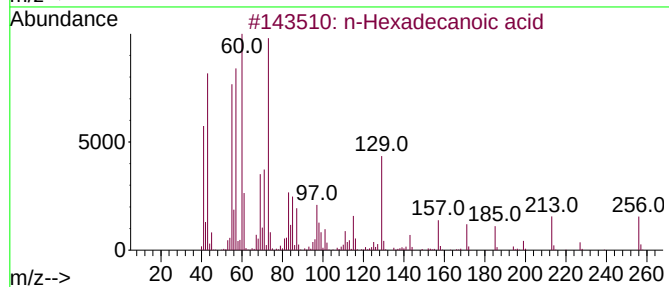
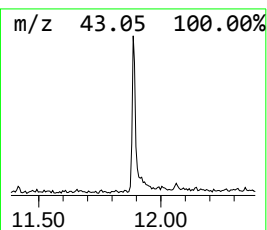
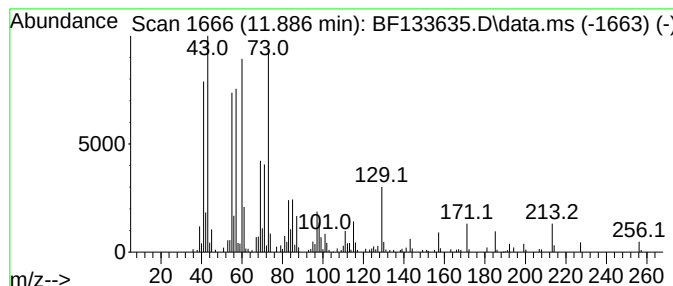
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
11.886	2.95 ng	200089	Phenanthrene-d10	11.363

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	87
4			Undecanoic acid	186	C11H22O2	000112-37-8	80
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060823\
Data File : BF133635.D
Acq On : 08 Jun 2023 11:25
Operator : CG\JU
Sample : 03016-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

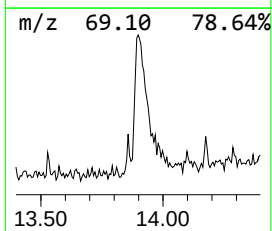
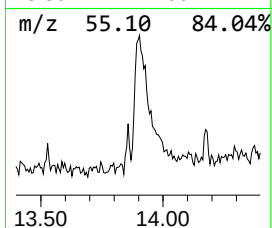
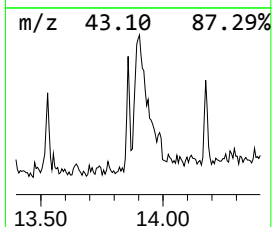
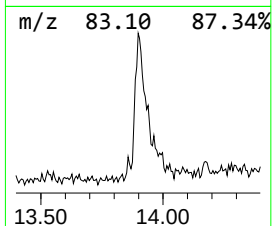
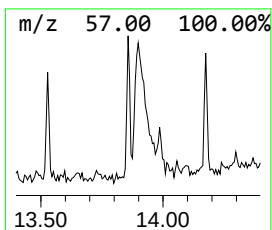
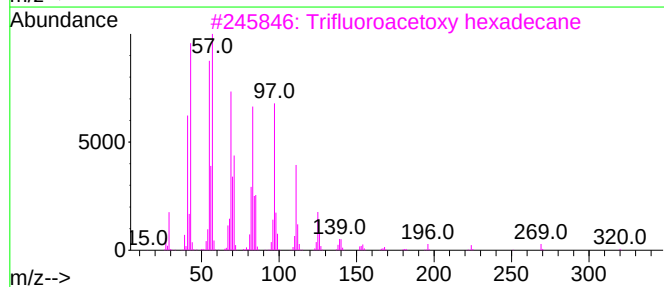
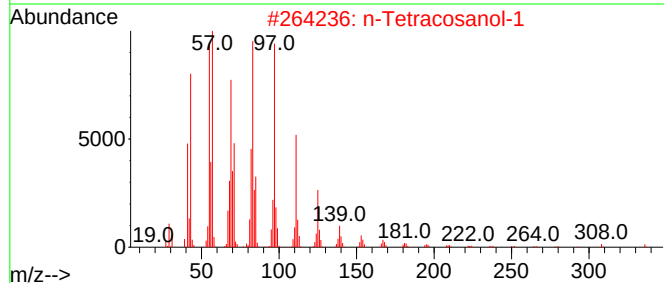
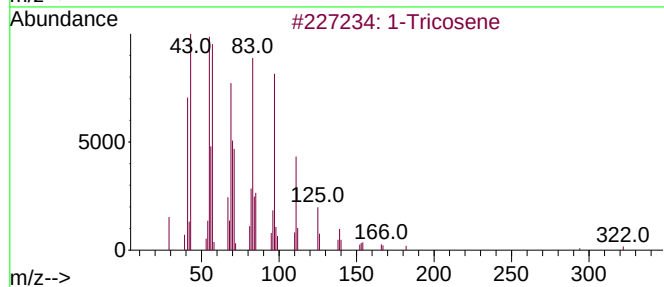
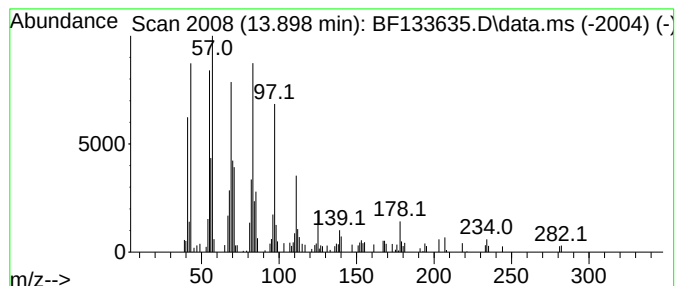
Instrument :
BNA_F
ClientSampleId :
SB28

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 1-Tricosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.898	4.39 ng	221106	Chrysene-d12	14.010	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene	322	C23H46	018835-32-0	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4	1-Octadecanol	270	C18H38O	000112-92-5	91
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060823\
Data File : BF133635.D
Acq On : 08 Jun 2023 11:25
Operator : CG\JU
Sample : 03016-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

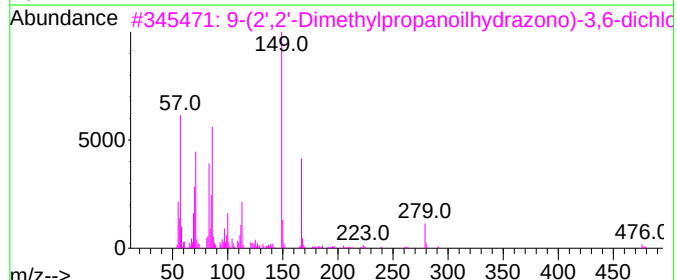
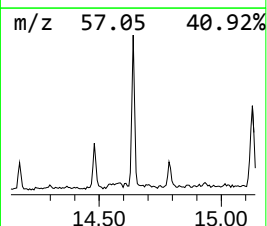
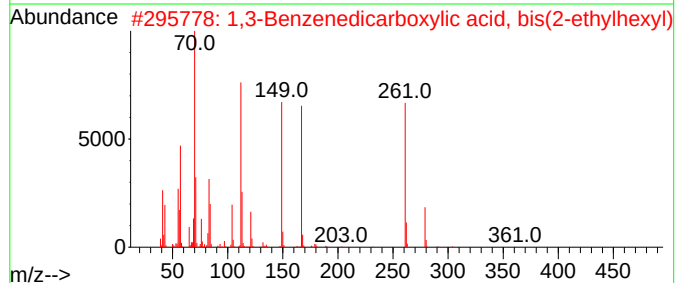
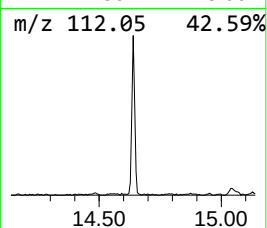
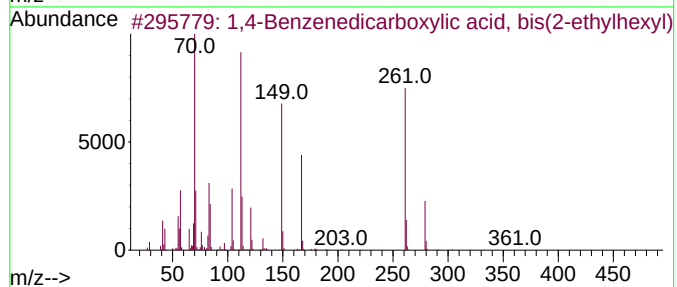
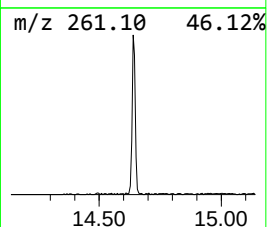
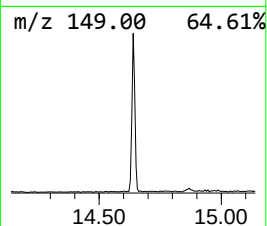
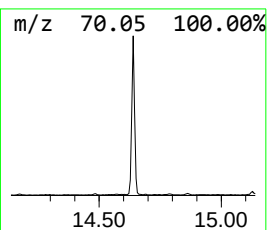
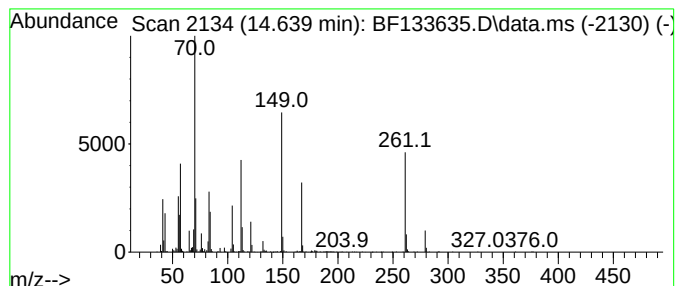
Instrument :
BNA_F
ClientSampleId :
SB28

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1,4-Benzenedicarboxylic aci... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.639	8.63 ng	434600	Chrysene-d12	14.010	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	64
2	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	52
3	9-(2',2'-Dimethylpropanoilhydraz...	576	C30H42Cl2N4O3	1000111-04-6	25
4	Phthalic acid, monodecyl ester	306	C18H26O4	024539-60-4	25
5	Phthalic acid, 3,5-difluoropheny...	320	C17H14F2O4	1000314-96-0	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060823\
Data File : BF133635.D
Acq On : 08 Jun 2023 11:25
Operator : CG\JU
Sample : 03016-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB28

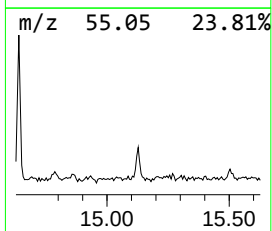
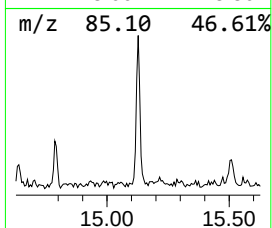
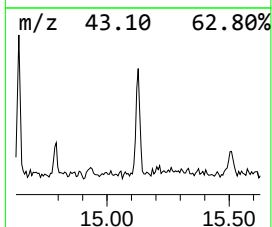
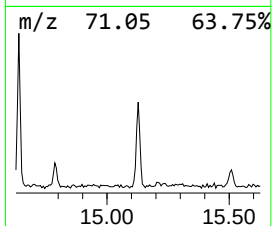
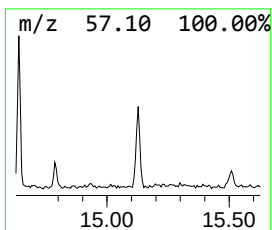
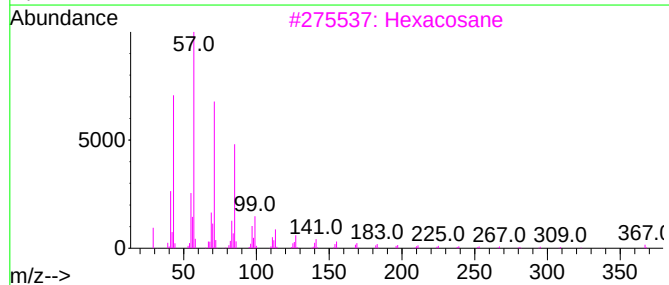
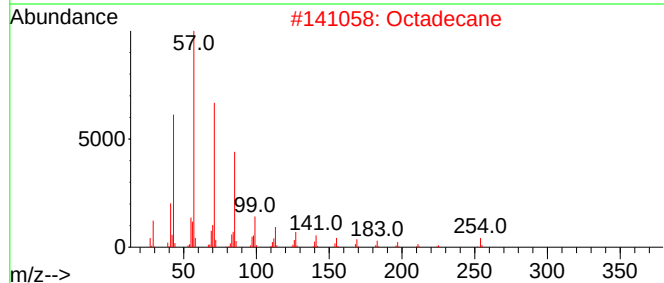
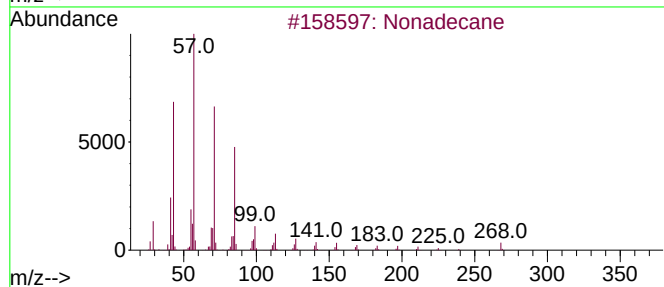
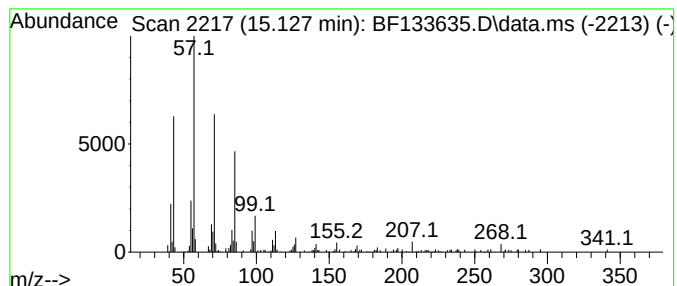
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.127	2.41 ng	106239	Perylene-d12	15.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	96
2			Octadecane	254	C18H38	000593-45-3	95
3			Hexacosane	366	C26H54	000630-01-3	90
4			Hentriacontane	437	C31H64	000630-04-6	90
5			Octacosane	394	C28H58	000630-02-4	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060823\
Data File : BF133635.D
Acq On : 08 Jun 2023 11:25
Operator : CG\JU
Sample : 03016-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB28

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.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
Benzophenone	10.586	5.3	ng	350814	3	9.875	1313960	20.0
n-Hexadecanoic ...	11.886	3.0	ng	200089	4	11.363	1354990	20.0
1-Tricosene	13.898	4.4	ng	221106	5	14.010	1007550	20.0
1,4-Benzenedica...	14.639	8.6	ng	434600	5	14.010	1007550	20.0
Nonadecane	15.127	2.4	ng	106239	6	15.474	882997	20.0