

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032621\
 Data File : BF123495.D
 Acq On : 26 Mar 2021 20:02
 Operator : JU/CG
 Sample : M1770-16
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-101I

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-BF032321.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123495.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.240	19	26	32	rVB	3357441	4466273	51.95%	8.494%
2	2.351	39	45	50	rVB2	100462	133315	1.55%	0.254%
3	2.610	78	89	95	rVB	235257	344084	4.00%	0.654%
4	2.740	106	111	120	rVB	251228	344294	4.00%	0.655%
5	4.657	431	437	441	rBV	708701	788588	9.17%	1.500%
6	5.122	508	516	524	rVB	86469	115650	1.35%	0.220%
7	5.516	579	583	587	rBV	3516356	3436655	39.98%	6.536%
8	6.516	749	753	759	rBV	2592708	2404747	27.97%	4.573%
9	6.898	814	818	821	rBV	1985085	1549239	18.02%	2.946%
10	7.463	907	914	917	rBV	4729012	5115108	59.50%	9.728%
11	7.563	921	931	941	rVB	308811	658375	7.66%	1.252%
12	8.186	1031	1037	1040	rBV	2148024	2035522	23.68%	3.871%
13	8.575	1097	1103	1115	rBV	498576	551927	6.42%	1.050%
14	9.263	1214	1220	1223	rBV	8533487	8596662	100.00%	16.349%
15	9.945	1331	1336	1339	rVB	2413692	2256085	26.24%	4.291%
16	10.139	1365	1369	1372	rBV	113860	91420	1.06%	0.174%
17	10.733	1464	1470	1473	rBV	5713986	5635671	65.56%	10.718%
18	11.433	1585	1589	1592	rBV	2539620	2167864	25.22%	4.123%
19	11.957	1672	1678	1683	rBV	284233	266048	3.09%	0.506%
20	13.027	1853	1860	1863	rBV	7848208	7500522	87.25%	14.264%
21	13.874	1999	2004	2007	rBV2	95062	135703	1.58%	0.258%
22	13.927	2007	2013	2023	rVV3	550827	1174676	13.66%	2.234%
23	14.080	2034	2039	2042	rBV	1511321	1400234	16.29%	2.663%
24	15.574	2288	2293	2298	rBV	1004991	1230940	14.32%	2.341%
25	16.151	2385	2391	2398	rBV6	62704	182806	2.13%	0.348%

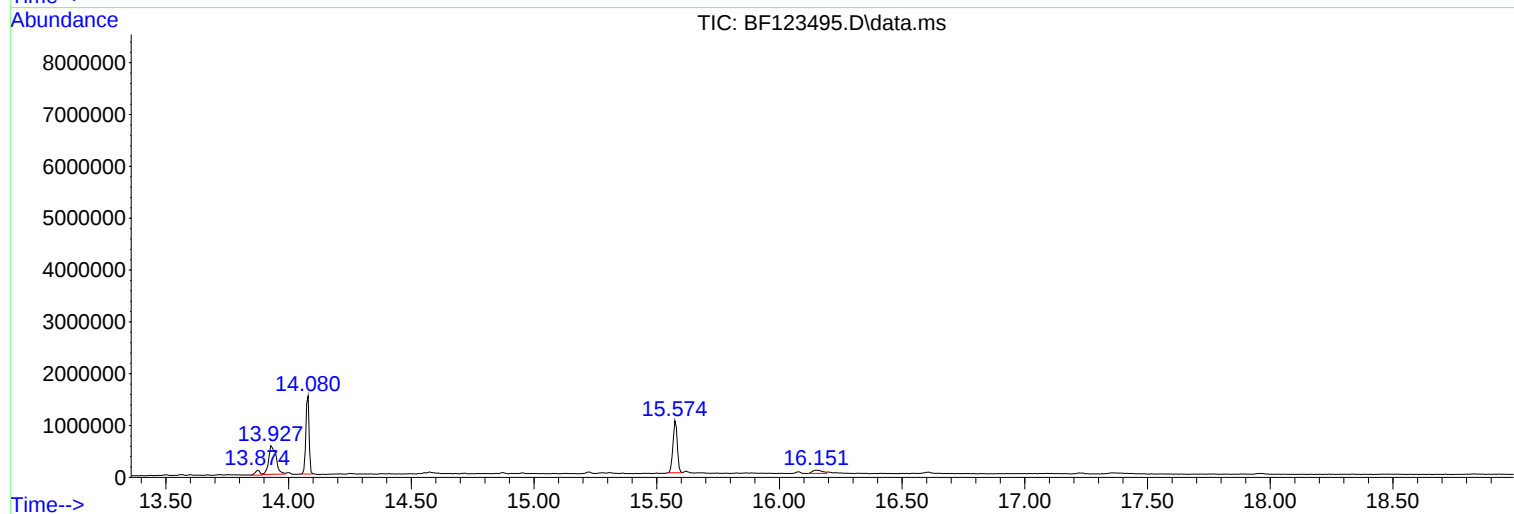
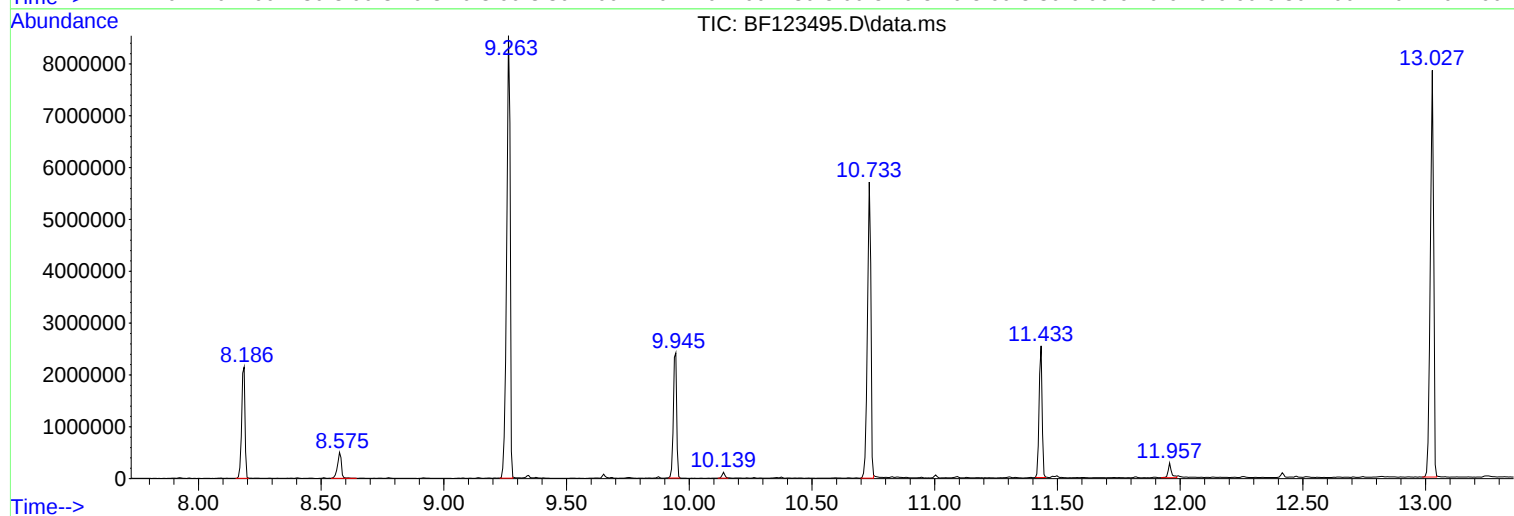
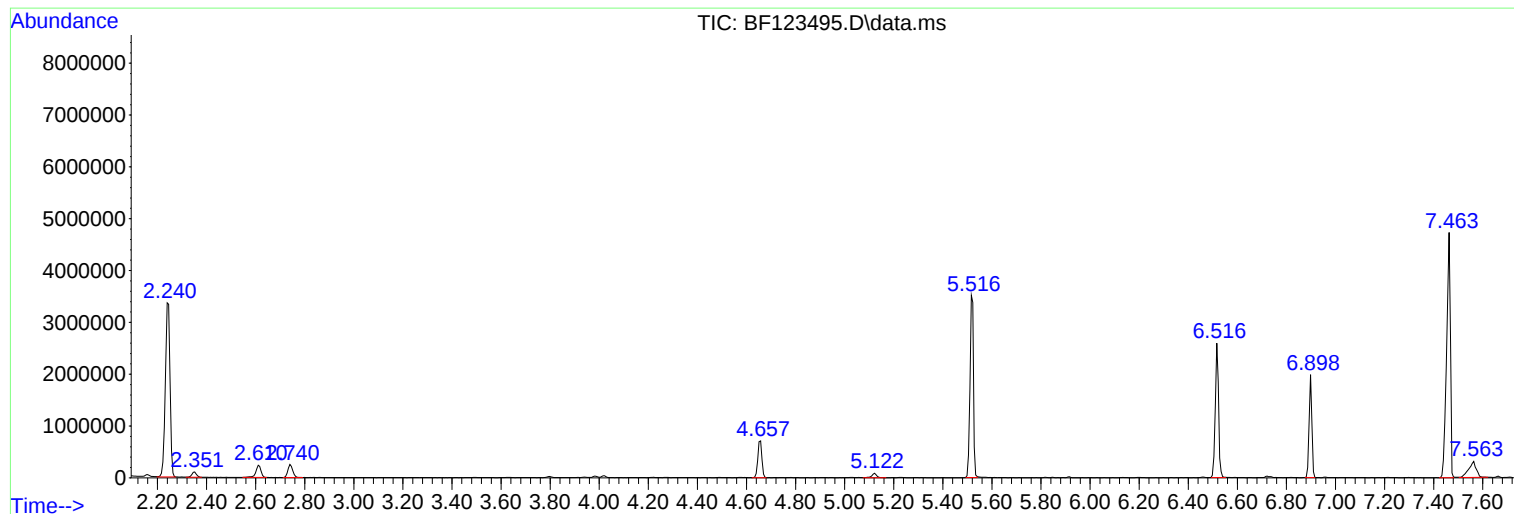
Sum of corrected areas: 52582408

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032621\
Data File : BF123495.D
Acq On : 26 Mar 2021 20:02
Operator : JU/CG
Sample : M1770-16
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-101I

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032621\
Data File : BF123495.D
Acq On : 26 Mar 2021 20:02
Operator : JU/CG
Sample : M1770-16
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-101I

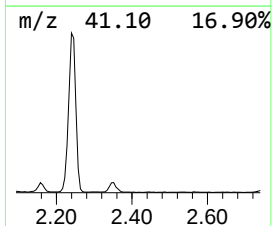
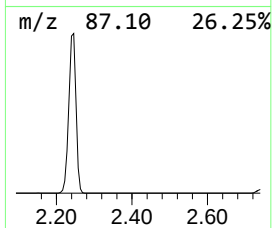
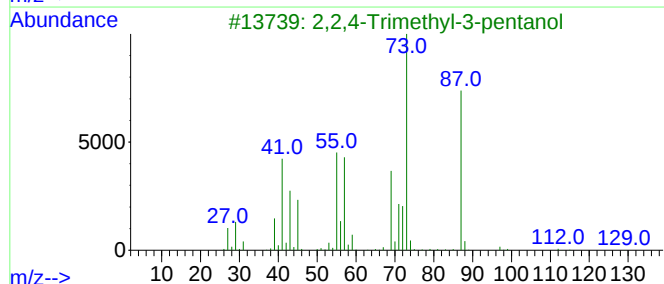
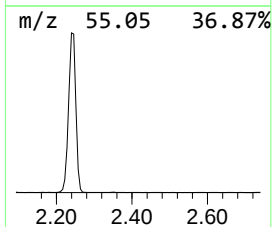
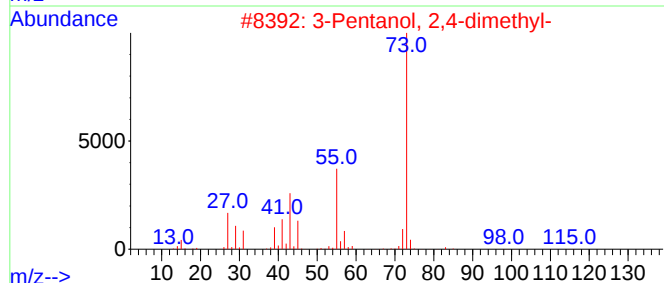
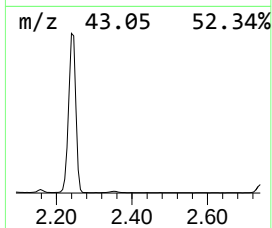
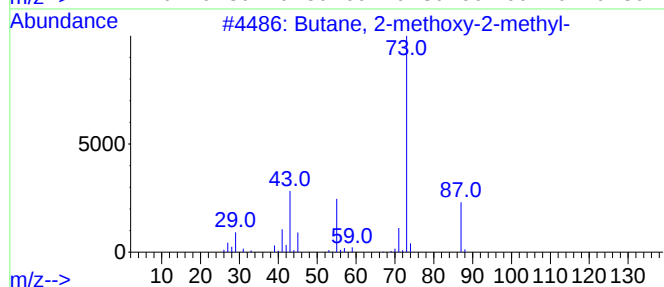
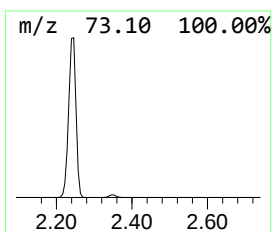
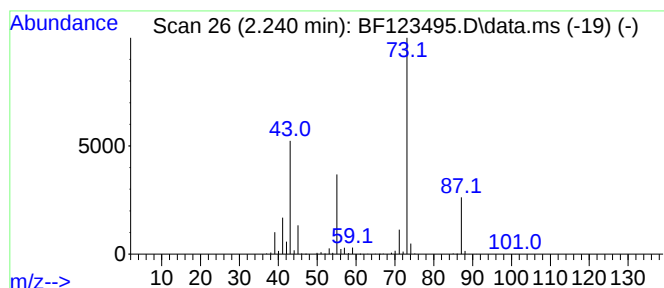
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.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.
2.240	57.66 ng	4466270	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032621\
Data File : BF123495.D
Acq On : 26 Mar 2021 20:02
Operator : JU/CG
Sample : M1770-16
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-101I

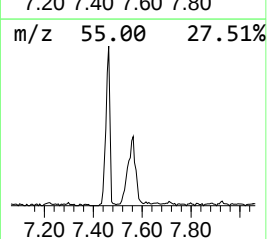
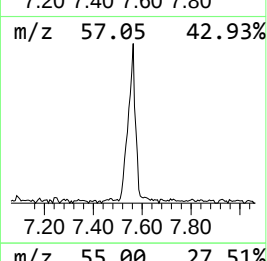
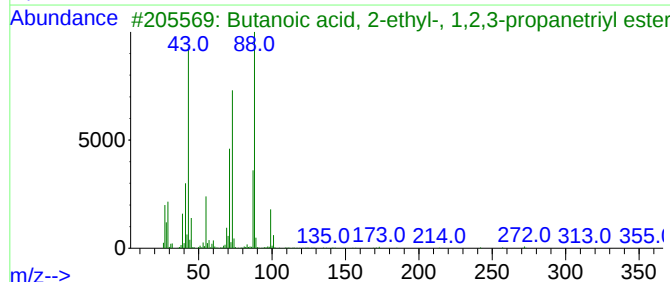
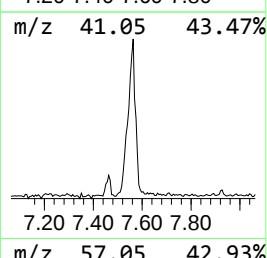
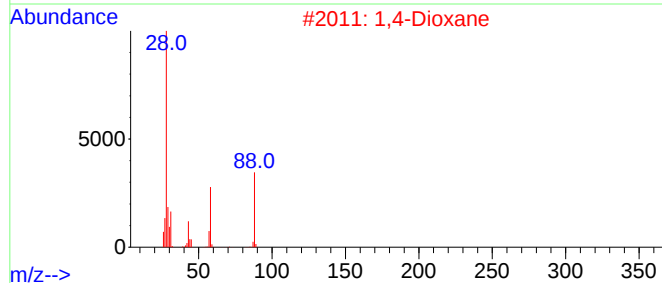
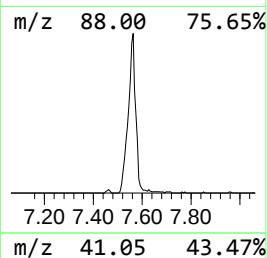
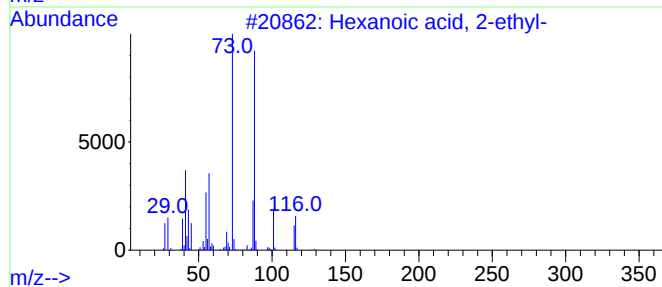
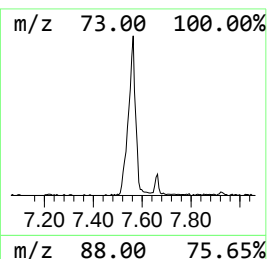
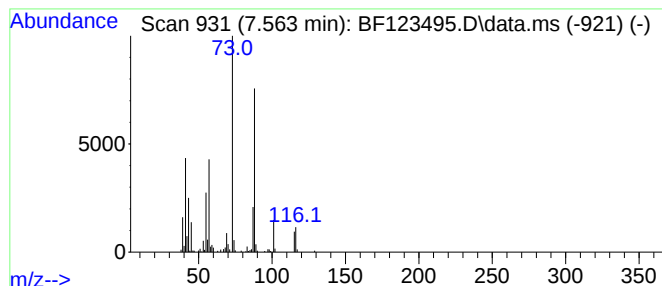
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexanoic acid, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.563	6.47 ng	658375	Naphthalene-d8	8.186

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2			1,4-Dioxane	88	C4H8O2	000123-91-1	47
3			Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	42
4			Propanoic acid, 3-hydroxy-2-meth...	118	C5H10O3	042998-03-8	40
5			Octanoic acid, 2-methyl-, methyl...	172	C10H20O2	002177-86-8	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032621\
Data File : BF123495.D
Acq On : 26 Mar 2021 20:02
Operator : JU/CG
Sample : M1770-16
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-101I

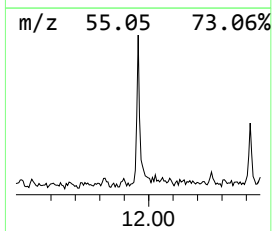
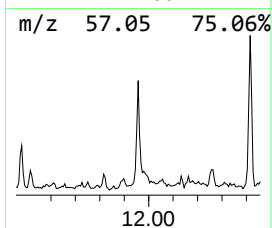
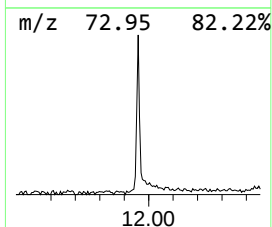
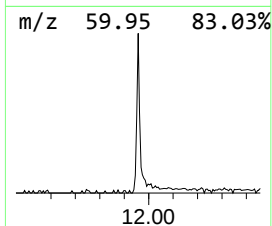
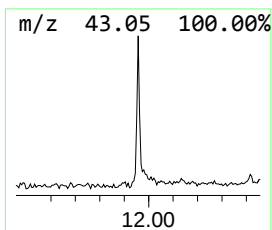
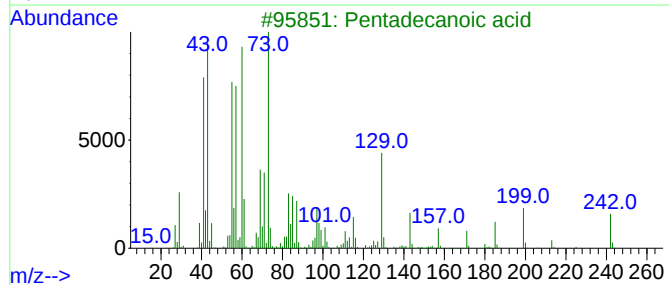
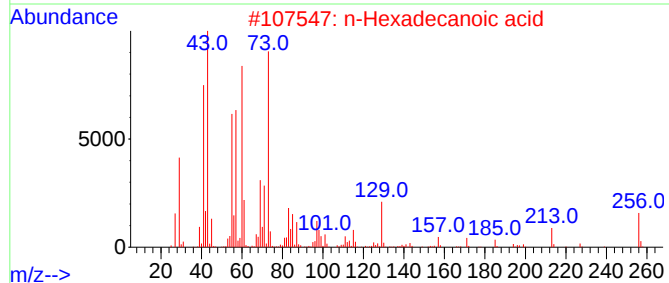
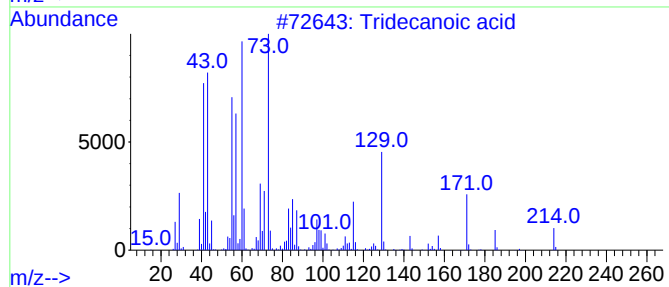
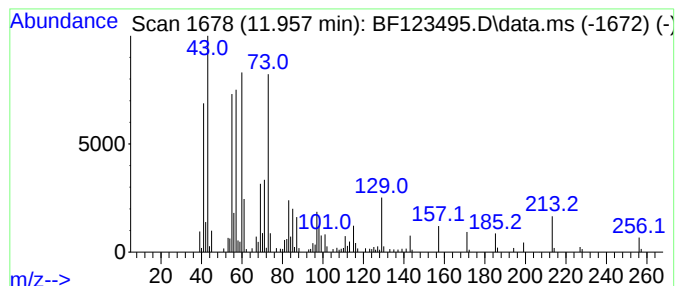
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tridecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	2.45 ng	266048	Phenanthrene-d10	11.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	95
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032621\
Data File : BF123495.D
Acq On : 26 Mar 2021 20:02
Operator : JU/CG
Sample : M1770-16
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-101I

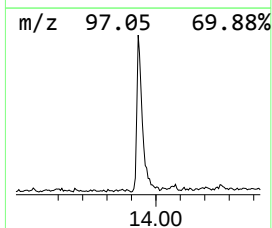
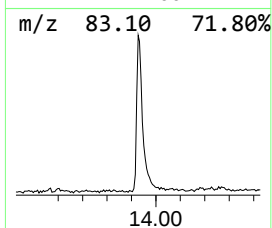
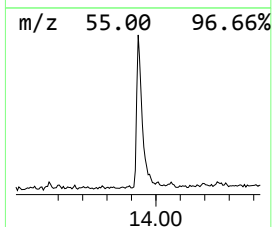
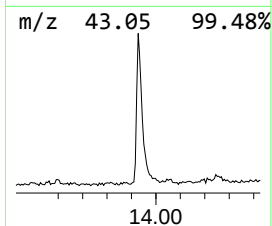
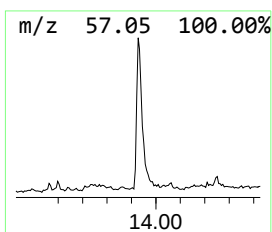
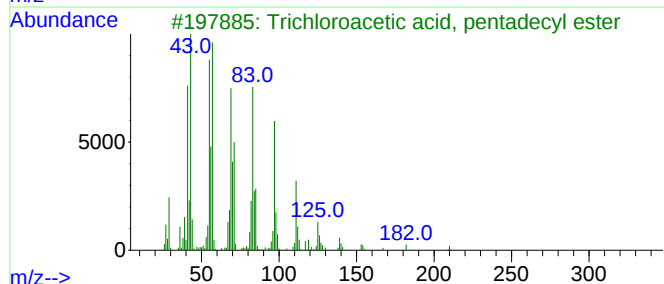
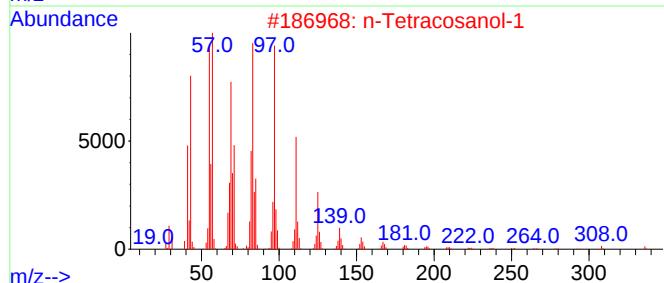
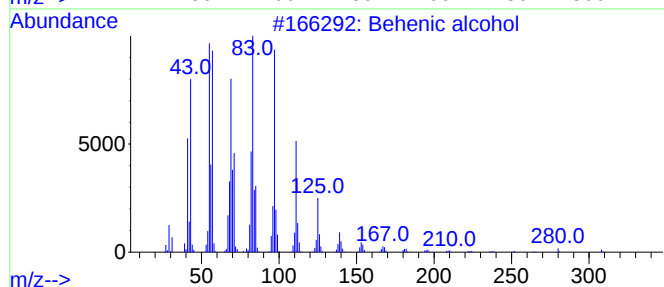
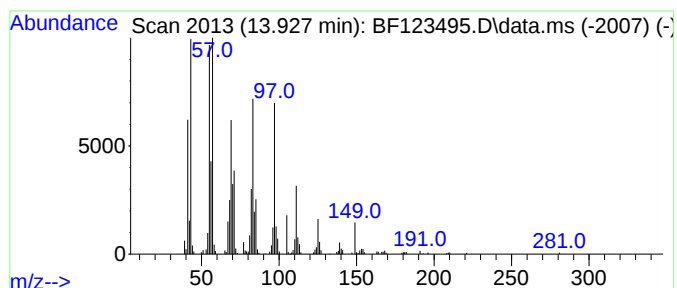
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Behenic alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.927	16.78 ng	1174680	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	93
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	93
3			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5			1-Heneicosanol	312	C21H44O	015594-90-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032621\
Data File : BF123495.D
Acq On : 26 Mar 2021 20:02
Operator : JU/CG
Sample : M1770-16
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-101I

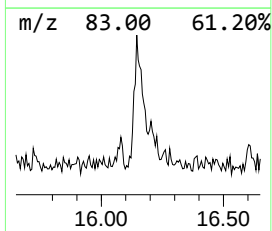
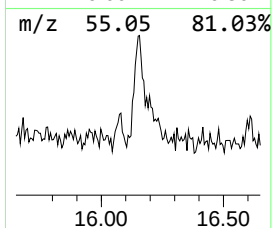
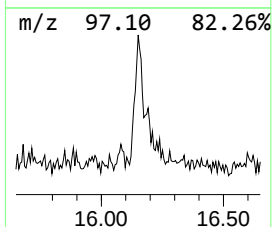
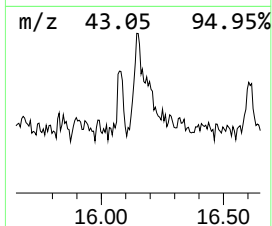
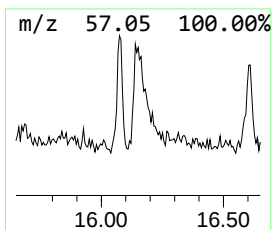
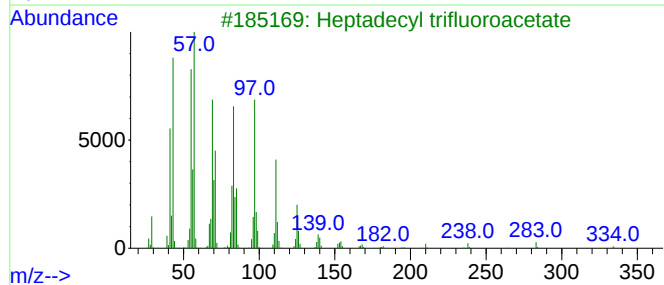
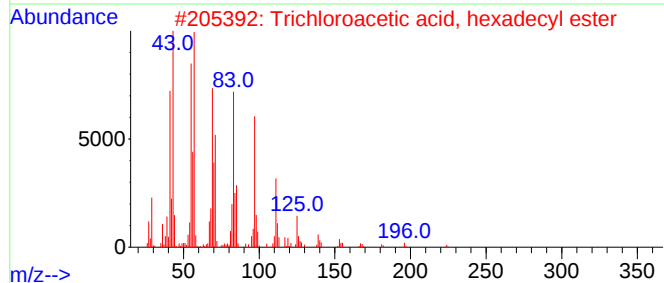
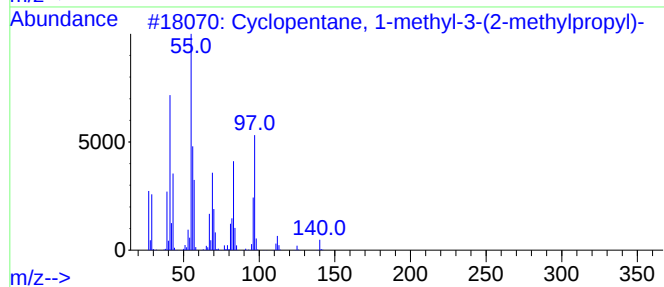
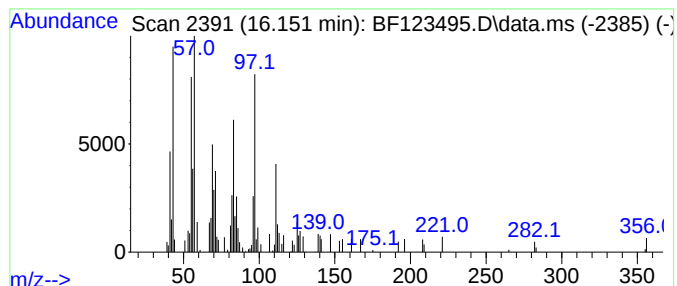
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Cyclopentane, 1-methyl-3-(2... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.151	2.97 ng	182806	Perylene-d12	15.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1-methyl-3-(2-meth...	140	C10H20	029053-04-1	70
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	60
3			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	58
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	58
5			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032621\
Data File : BF123495.D
Acq On : 26 Mar 2021 20:02
Operator : JU/CG
Sample : M1770-16
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-101I

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.240	57.7	ng	4466270	1	6.898	1549240	20.0
Hexanoic acid, ...	7.563	6.5	ng	658375	2	8.186	2035520	20.0
Tridecanoic acid	11.957	2.5	ng	266048	4	11.433	2167860	20.0
Behenic alcohol	13.927	16.8	ng	1174680	5	14.080	1400230	20.0
Cyclopentane, 1...	16.151	3.0	ng	182806	6	15.574	1230940	20.0