

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081222\
 Data File : BF129748.D
 Acq On : 12 Aug 2022 17:15
 Operator : CG\JU
 Sample : N4154-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WV-TOTECOMP-1

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-BF072522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129748.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.675	401	406	410	rVB	43588	47450	1.14%	0.224%
2	5.469	538	541	558	rBV	1744069	1860521	44.83%	8.793%
3	6.487	710	714	722	rBV	1075213	1088223	26.22%	5.143%
4	6.828	769	772	776	rBV	893355	711985	17.16%	3.365%
5	7.398	864	869	872	rBV	2548309	2409722	58.07%	11.388%
6	8.110	987	990	994	rVB	1066647	855441	20.61%	4.043%
7	8.269	1013	1017	1021	rVB	329289	252740	6.09%	1.194%
8	8.345	1026	1030	1036	rBV2	77200	120710	2.91%	0.570%
9	9.186	1168	1173	1176	rBV	4828474	4149876	100.00%	19.612%
10	9.869	1285	1289	1292	rBV	1039960	846983	20.41%	4.003%
11	10.080	1321	1325	1329	rBV	54880	50554	1.22%	0.239%
12	10.663	1420	1424	1427	rBV	2417556	2071650	49.92%	9.791%
13	11.357	1538	1542	1546	rBV	876505	713825	17.20%	3.374%
14	11.874	1627	1630	1639	rBV2	130964	166223	4.01%	0.786%
15	12.663	1761	1764	1772	rBV2	180810	207081	4.99%	0.979%
16	12.945	1807	1812	1815	rBV	3904027	3480347	83.87%	16.448%
17	13.880	1965	1971	1982	rBV2	65886	180092	4.34%	0.851%
18	14.010	1989	1993	1996	rBV	744587	722824	17.42%	3.416%
19	14.098	2004	2008	2013	rVB	106463	106859	2.57%	0.505%
20	15.080	2172	2175	2180	rVB3	46797	70697	1.70%	0.334%
21	15.480	2236	2243	2250	rVB	661657	852450	20.54%	4.029%
22	15.892	2309	2313	2318	rVB2	66930	99735	2.40%	0.471%
23	16.386	2394	2397	2404	rVB2	58430	93524	2.25%	0.442%

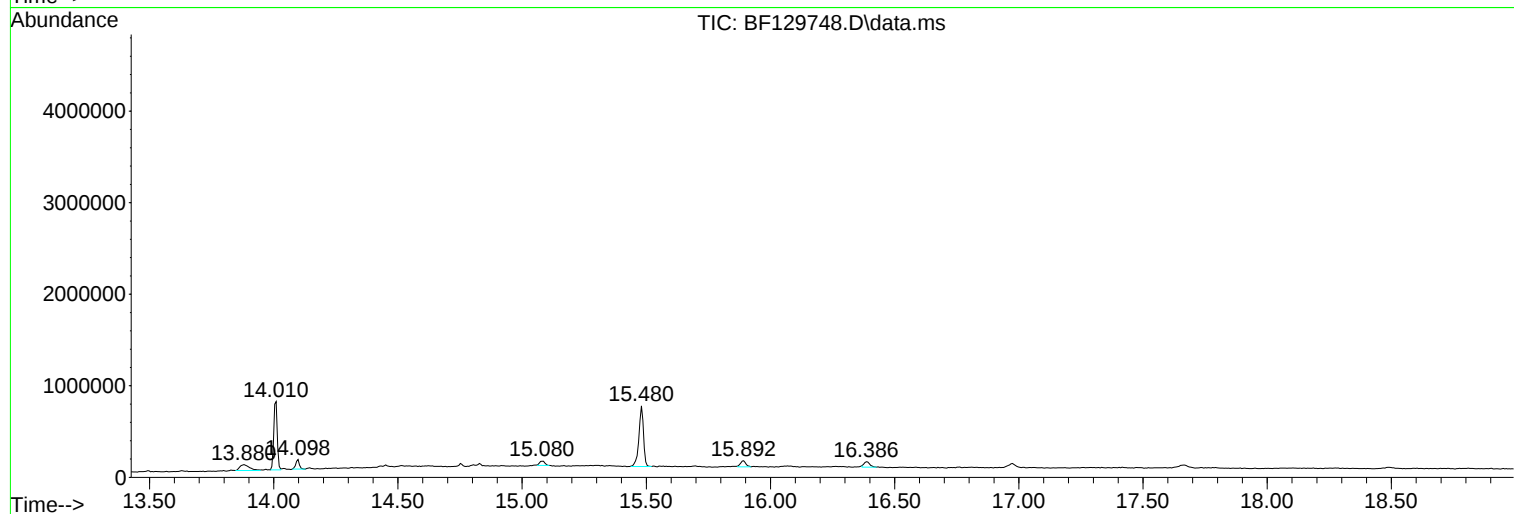
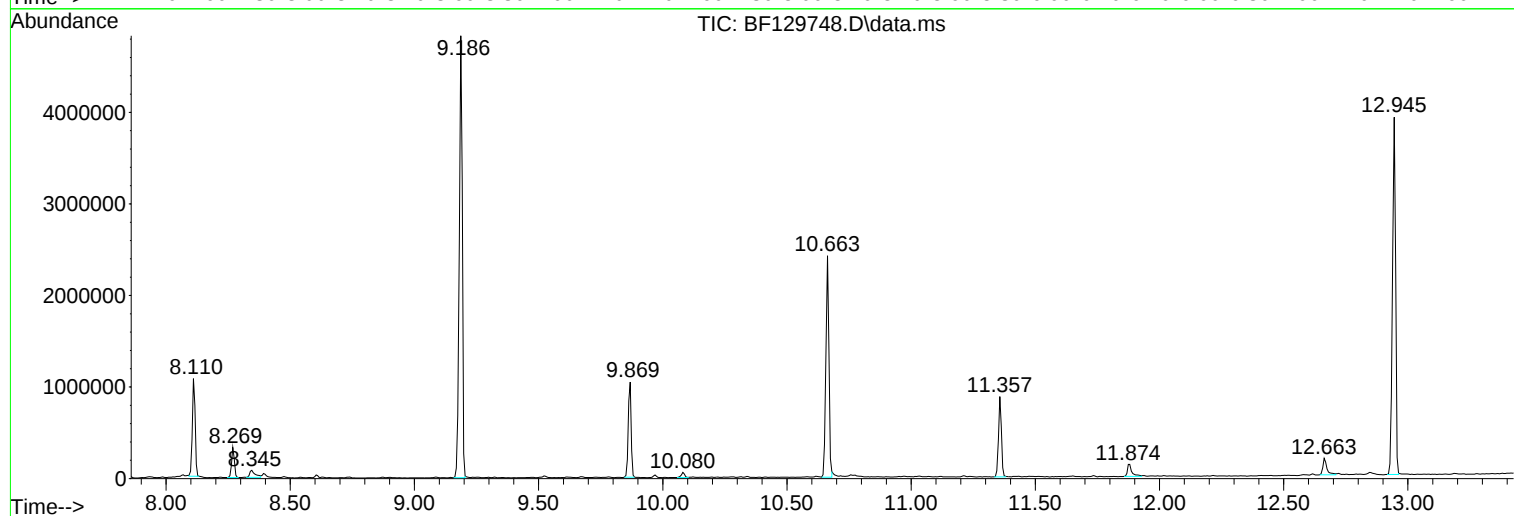
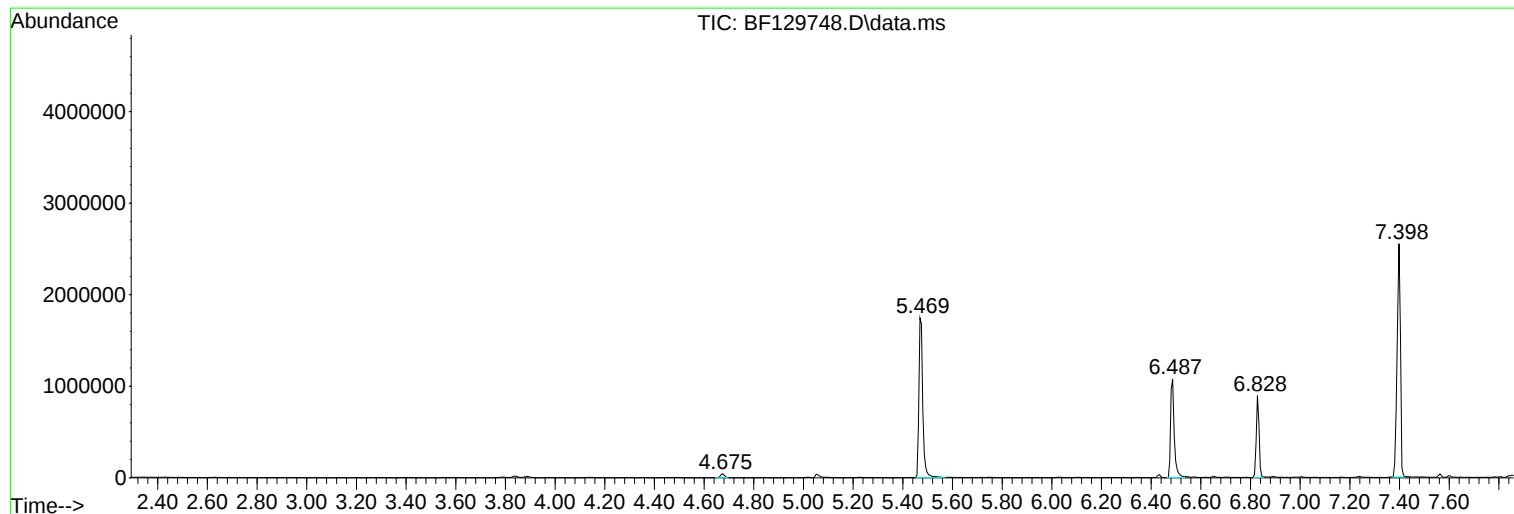
Sum of corrected areas: 21159512

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081222\
Data File : BF129748.D
Acq On : 12 Aug 2022 17:15
Operator : CG\JU
Sample : N4154-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WV-TOTECOMP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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\BF081222\
Data File : BF129748.D
Acq On : 12 Aug 2022 17:15
Operator : CG\JU
Sample : N4154-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WV-TOTECOMP-1

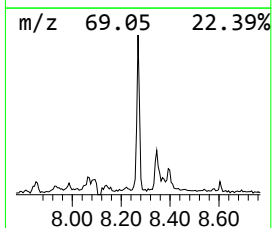
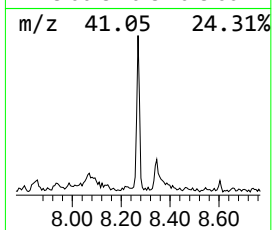
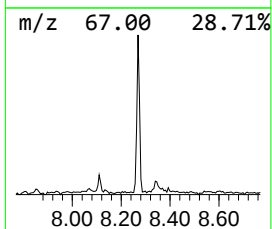
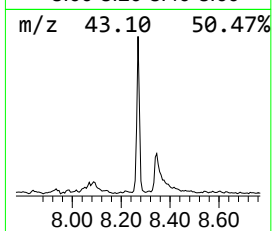
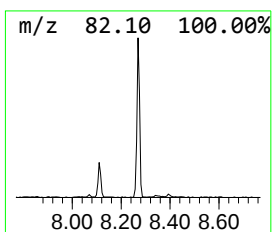
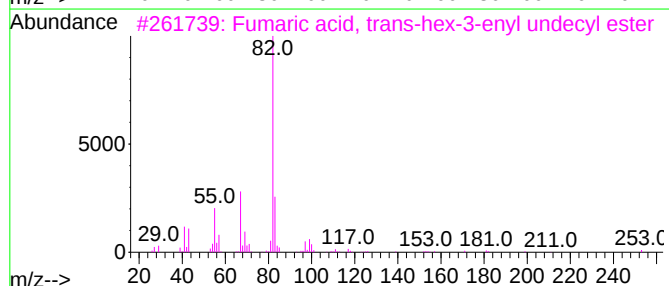
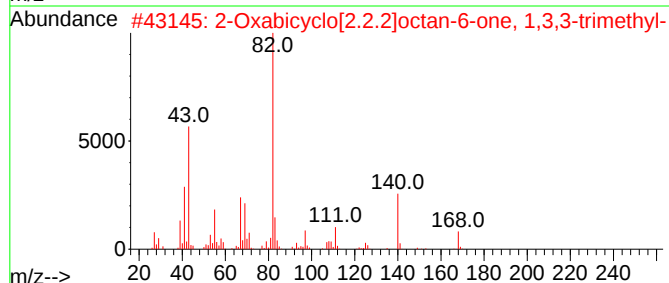
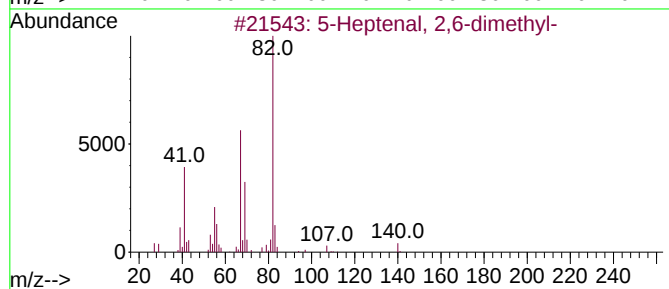
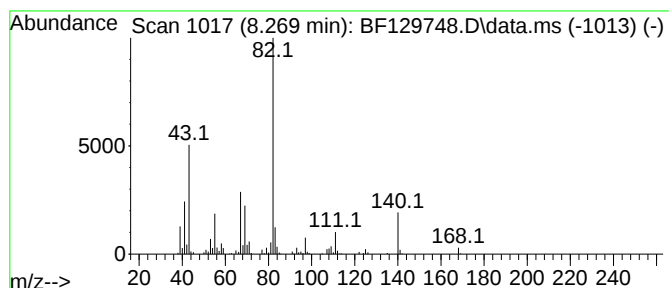
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 5-Heptenal, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.269	5.91 ng	252740	Naphthalene-d8	8.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Heptenal, 2,6-dimethyl-	140	C9H16O	000106-72-9	80
2			2-Oxabicyclo[2.2.2]octan-6-one, ...	168	C10H16O2	107598-08-3	78
3			Fumaric acid, trans-hex-3-enyl u...	352	C21H36O4	1000348-89-1	50
4			Fumaric acid, cis-hex-3-enyl non...	324	C19H32O4	1000348-86-5	40
5			Fumaric acid, cis-hex-3-enyl dod...	366	C22H38O4	1000348-86-7	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081222\
Data File : BF129748.D
Acq On : 12 Aug 2022 17:15
Operator : CG\JU
Sample : N4154-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WV-TOTECOMP-1

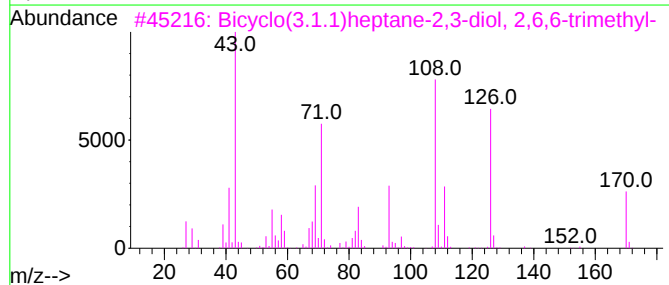
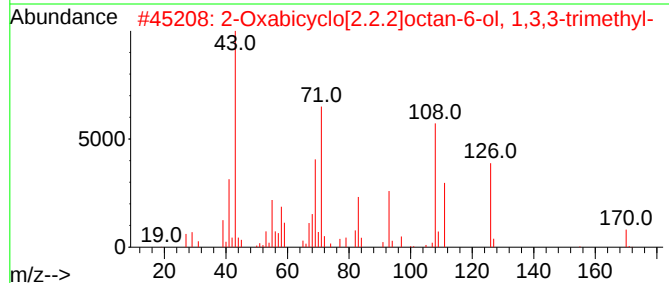
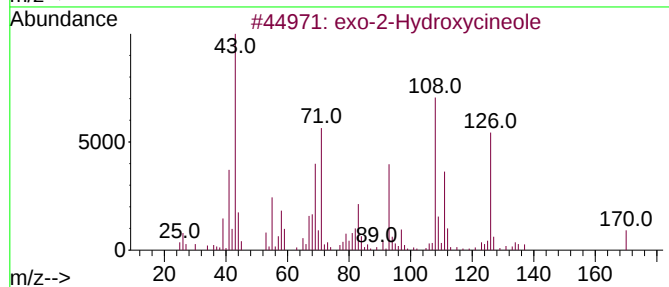
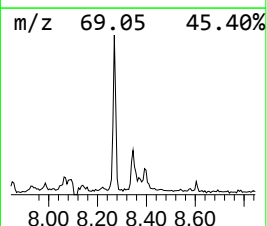
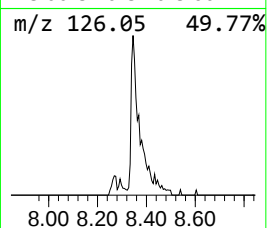
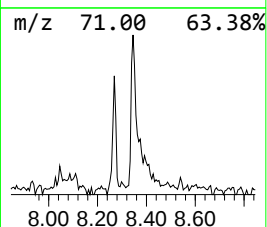
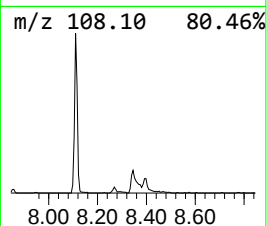
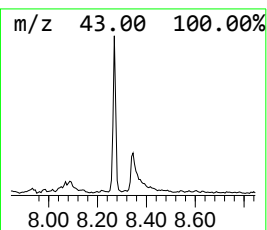
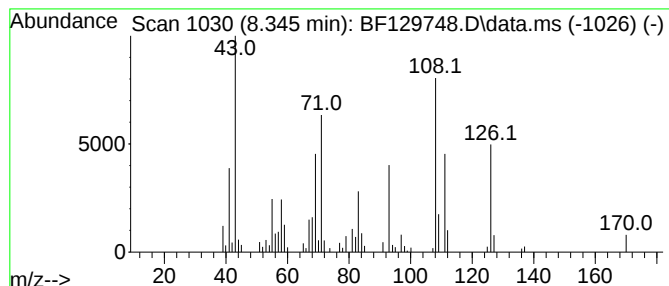
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 exo-2-Hydroxycineole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.345	2.82 ng	120710	Naphthalene-d8	8.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			exo-2-Hydroxycineole	170	C10H18O2	092999-78-5	96
2			2-Oxabicyclo[2.2.2]octan-6-ol, 1...	170	C10H18O2	018679-48-6	94
3			Bicyclo(3.1.1)heptane-2,3-diol, ...	170	C10H18O2	053404-49-2	78
4			2-Oxabicyclo[2.2.2]octan-6-ol, 1...	212	C12H20O3	057709-95-2	56
5			9,9-Dimethyl-2-oxabicyclo[4.2.1]...	168	C10H16O2	1000443-06-4	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081222\
Data File : BF129748.D
Acq On : 12 Aug 2022 17:15
Operator : CG\JU
Sample : N4154-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WV-TOTECOMP-1

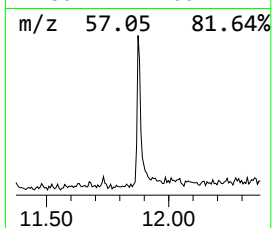
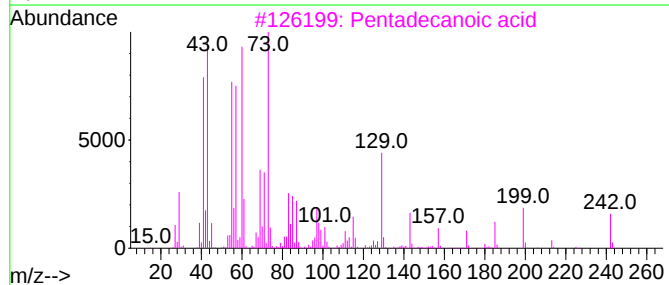
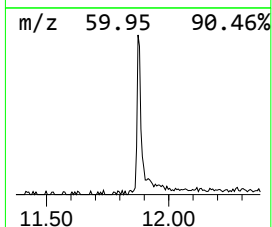
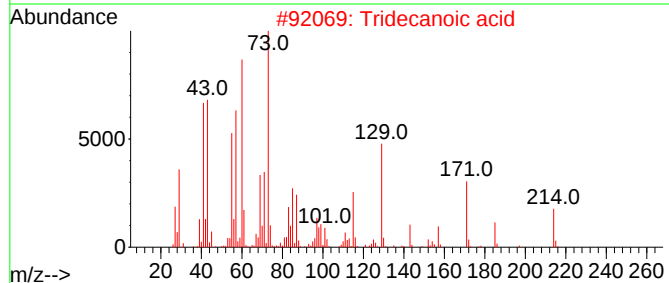
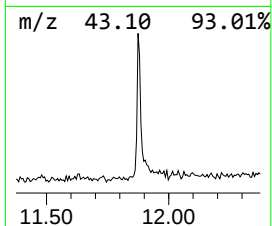
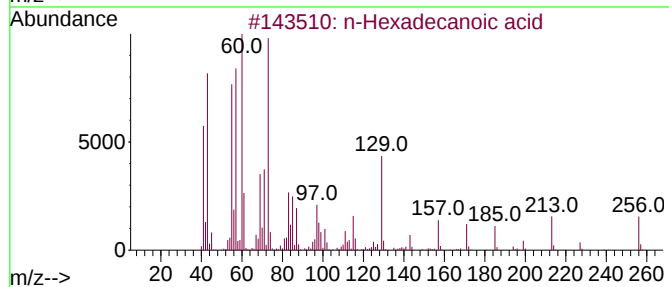
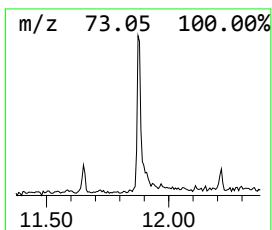
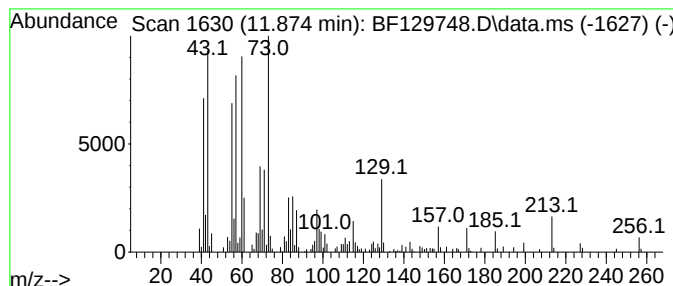
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.874	4.66 ng	166223	Phenanthrene-d10	11.357

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	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			Nonanoic acid	158	C9H18O2	000112-05-0	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081222\
Data File : BF129748.D
Acq On : 12 Aug 2022 17:15
Operator : CG\JU
Sample : N4154-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WV-TOTECOMP-1

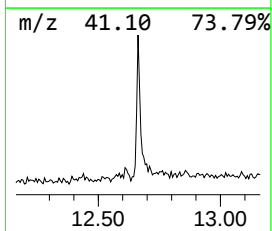
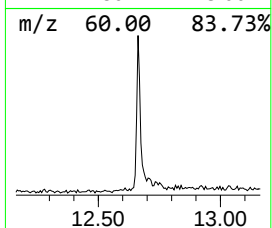
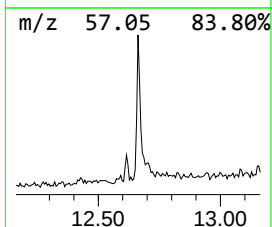
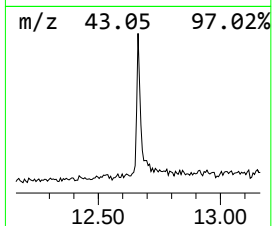
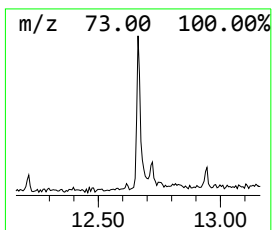
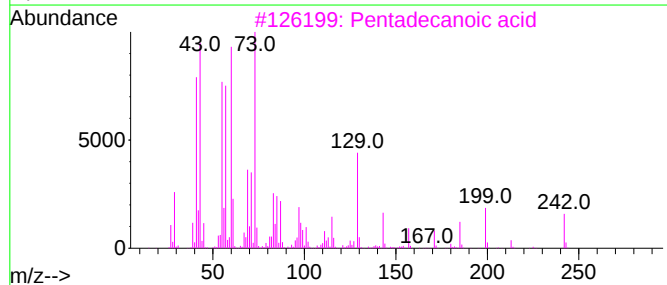
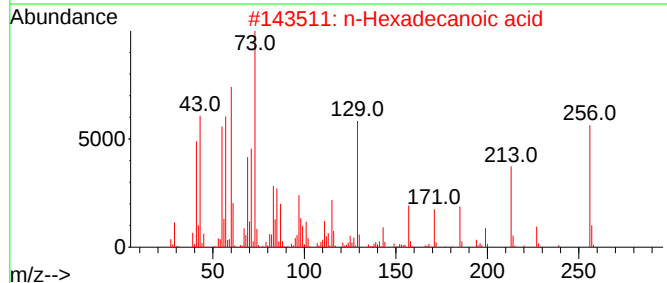
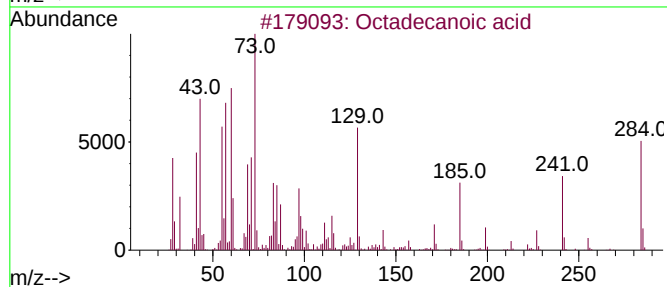
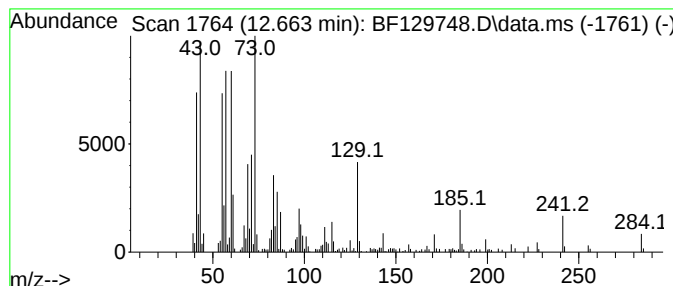
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.663	5.80 ng	207081	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081222\
Data File : BF129748.D
Acq On : 12 Aug 2022 17:15
Operator : CG\JU
Sample : N4154-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WV-TOTECOMP-1

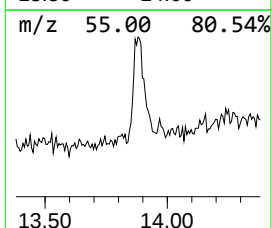
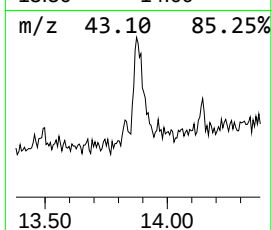
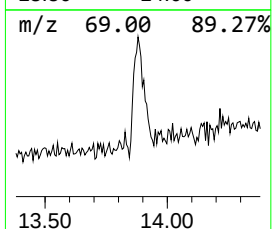
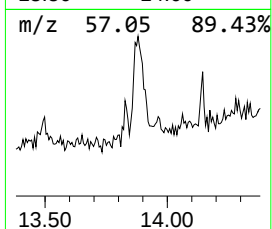
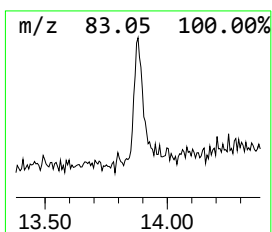
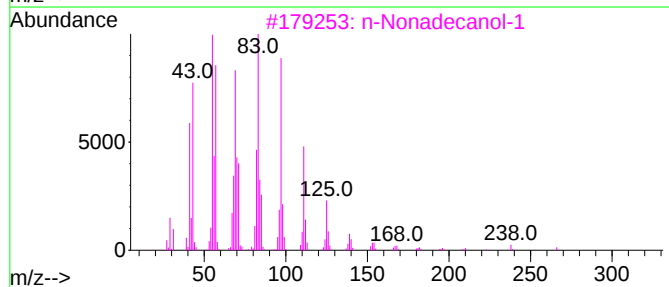
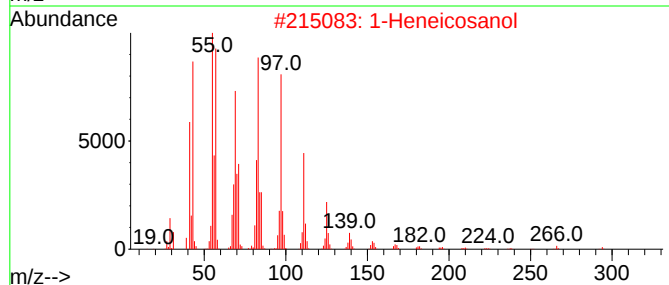
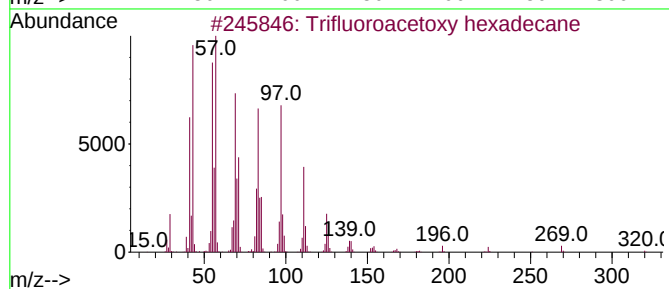
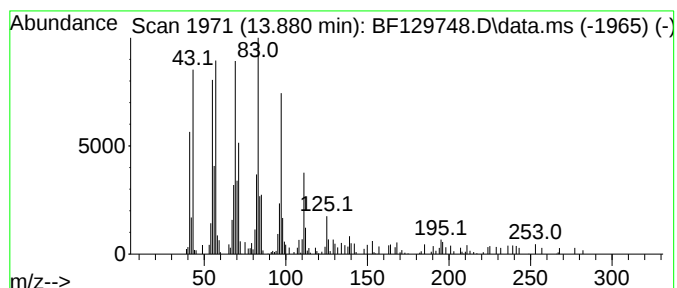
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	4.98 ng	180092	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2			1-Heneicosanol	312	C21H44O	015594-90-8	93
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	93
4			1-Tetracosene	336	C24H48	010192-32-2	91
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081222\
Data File : BF129748.D
Acq On : 12 Aug 2022 17:15
Operator : CG\JU
Sample : N4154-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WV-TOTECOMP-1

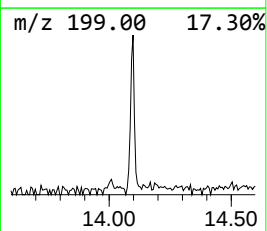
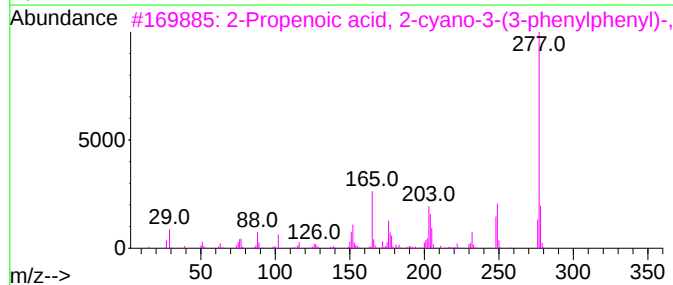
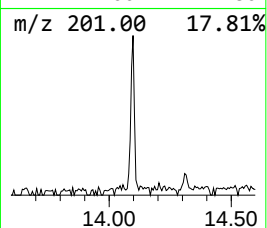
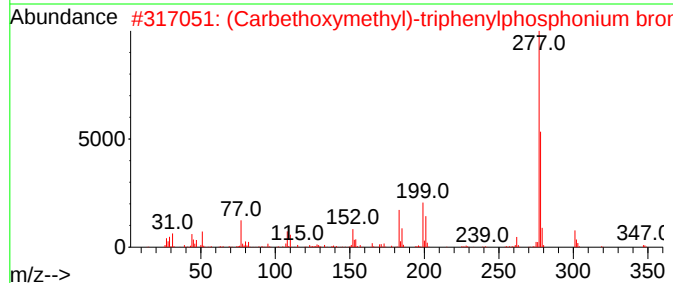
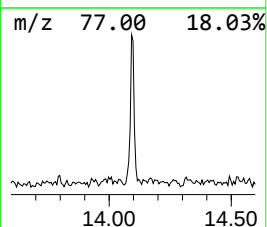
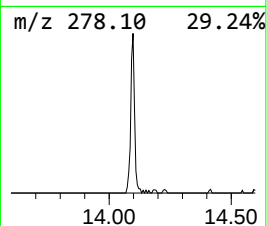
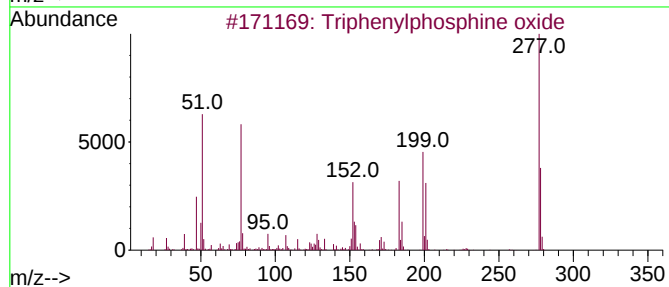
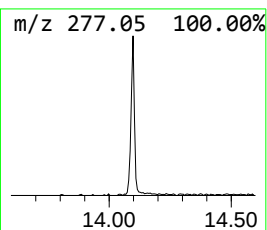
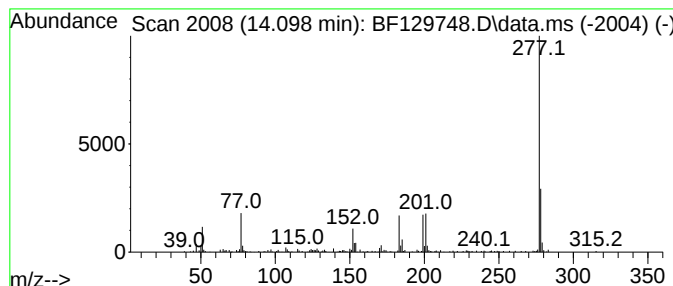
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.098	2.96 ng	106859	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	64
3			2-Propenoic acid, 2-cyano-3-(3-p...	277	C18H15NO2	1000080-00-3	59
4			(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19N03S	1000483-83-4	50
5			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081222\
Data File : BF129748.D
Acq On : 12 Aug 2022 17:15
Operator : CG\JU
Sample : N4154-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WV-TOTECOMP-1

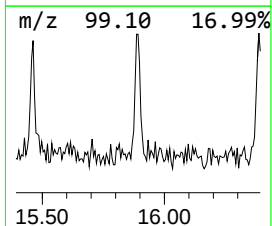
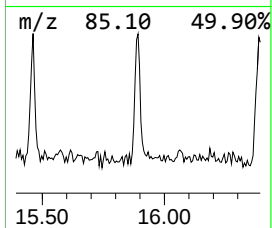
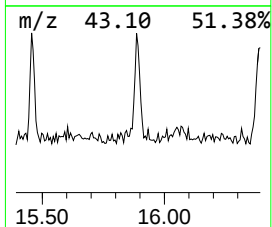
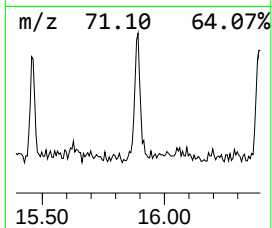
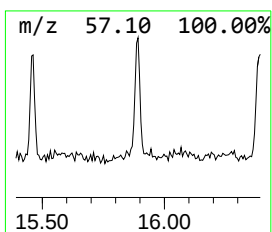
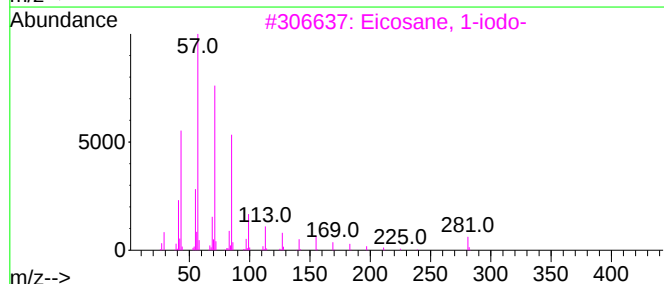
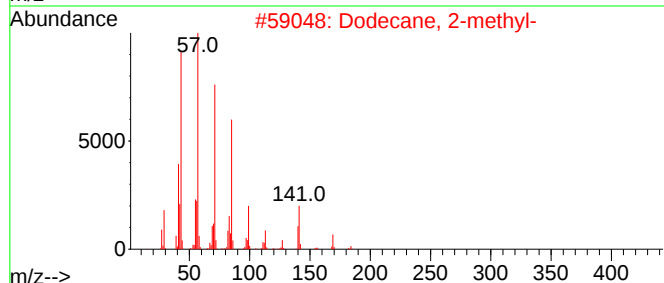
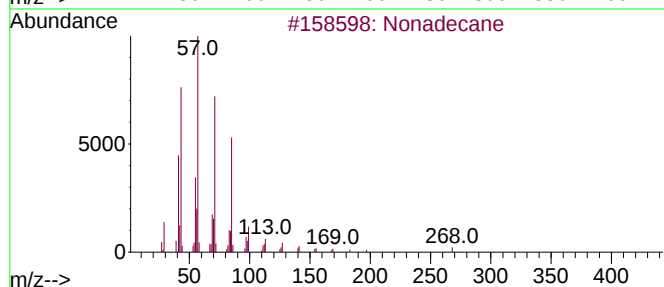
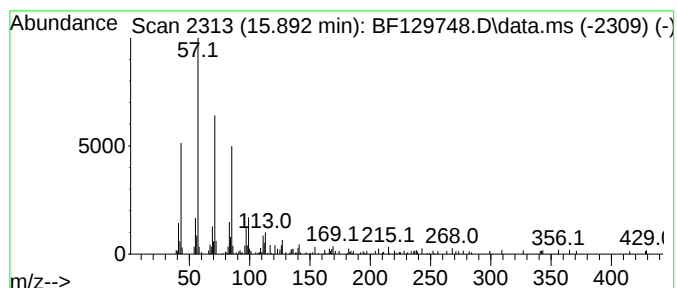
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.892	2.34 ng	99735	Perylene-d12	15.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	91
2			Dodecane, 2-methyl-	184	C13H28	001560-97-0	90
3			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	87
4			Octacosane	394	C28H58	000630-02-4	86
5			Tetratetracontane	619	C44H90	007098-22-8	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081222\
Data File : BF129748.D
Acq On : 12 Aug 2022 17:15
Operator : CG\JU
Sample : N4154-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WV-TOTECOMP-1

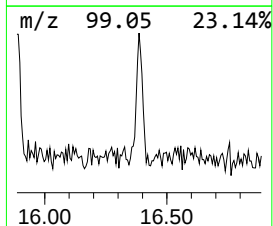
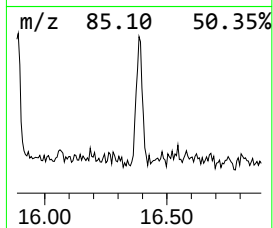
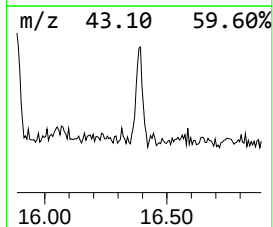
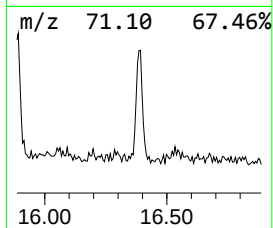
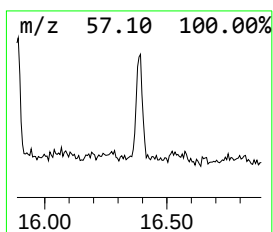
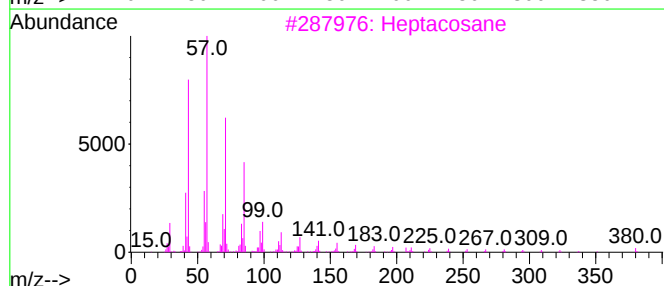
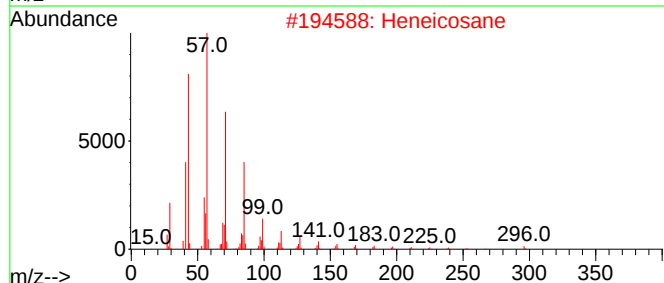
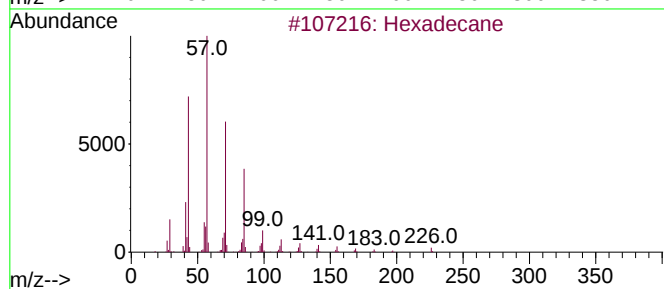
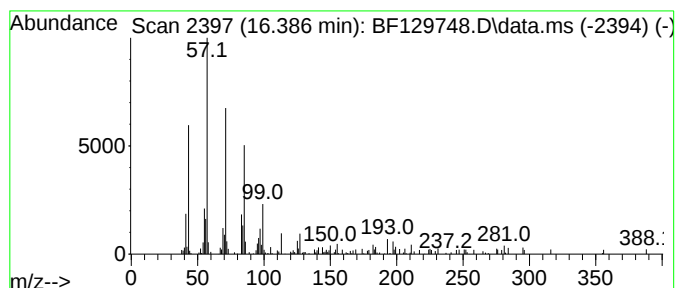
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.386	2.19 ng	93524	Perylene-d12	15.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	94
2			Heneicosane	296	C21H44	000629-94-7	93
3			Heptacosane	380	C27H56	000593-49-7	86
4			5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	86
5			Pentadecane, 2-methyl-	226	C16H34	001560-93-6	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081222\
Data File : BF129748.D
Acq On : 12 Aug 2022 17:15
Operator : CG\JU
Sample : N4154-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WV-TOTECOMP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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
5-Heptenal, 2,6...	8.269	5.9	ng	252740	2	8.110	855441	20.0
exo-2-Hydroxyci...	8.345	2.8	ng	120710	2	8.110	855441	20.0
n-Hexadecanoic ...	11.874	4.7	ng	166223	4	11.357	713825	20.0
Octadecanoic acid	12.663	5.8	ng	207081	4	11.357	713825	20.0
Trifluoroacetox...	13.880	5.0	ng	180092	5	14.010	722824	20.0
Triphenylphosph...	14.098	3.0	ng	106859	5	14.010	722824	20.0
Nonadecane	15.892	2.3	ng	99735	6	15.480	852450	20.0
Hexadecane	16.386	2.2	ng	93524	6	15.480	852450	20.0