

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062223\
 Data File : BF133900.D
 Acq On : 22 Jun 2023 14:28
 Operator : CG\JU
 Sample : 03321-13
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-21

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-BF060923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133900.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	15	rVB	372293	480965	25.40%	3.234%
2	2.240	22	26	37	rVB2	22476	36520	1.93%	0.246%
3	5.093	505	511	520	rBV	753074	873673	46.13%	5.874%
4	5.493	574	579	582	rBV	1820157	1603072	84.64%	10.778%
5	5.881	641	645	650	rBV	44807	40252	2.13%	0.271%
6	6.493	744	749	752	rBV	1869892	1590139	83.96%	10.691%
7	6.857	808	811	815	rBV	787624	616466	32.55%	4.145%
8	7.416	902	906	918	rBV	1149625	1089747	57.54%	7.326%
9	8.139	1025	1029	1032	rBV	889233	774703	40.90%	5.208%
10	9.216	1208	1212	1215	rBV	2243181	1893926	100.00%	12.733%
11	9.892	1324	1327	1331	rBV	924794	806138	42.56%	5.420%
12	10.610	1446	1449	1457	rVB	132182	107129	5.66%	0.720%
13	10.686	1458	1462	1472	rVV	1281781	1124985	59.40%	7.563%
14	11.386	1578	1581	1589	rBV	809777	750059	39.60%	5.043%
15	11.916	1668	1671	1683	rBV2	131156	141275	7.46%	0.950%
16	12.710	1803	1806	1810	rBV3	25909	31038	1.64%	0.209%
17	12.986	1848	1853	1856	rBV	1691376	1490002	78.67%	10.017%
18	13.563	1947	1951	1954	rBV2	19581	23866	1.26%	0.160%
19	13.898	2004	2008	2018	rBV2	72379	164326	8.68%	1.105%
20	14.045	2029	2033	2037	rBV	672730	640931	33.84%	4.309%
21	15.192	2225	2228	2233	rVB2	49359	56020	2.96%	0.377%
22	15.557	2285	2290	2294	rBV	425112	538936	28.46%	3.623%

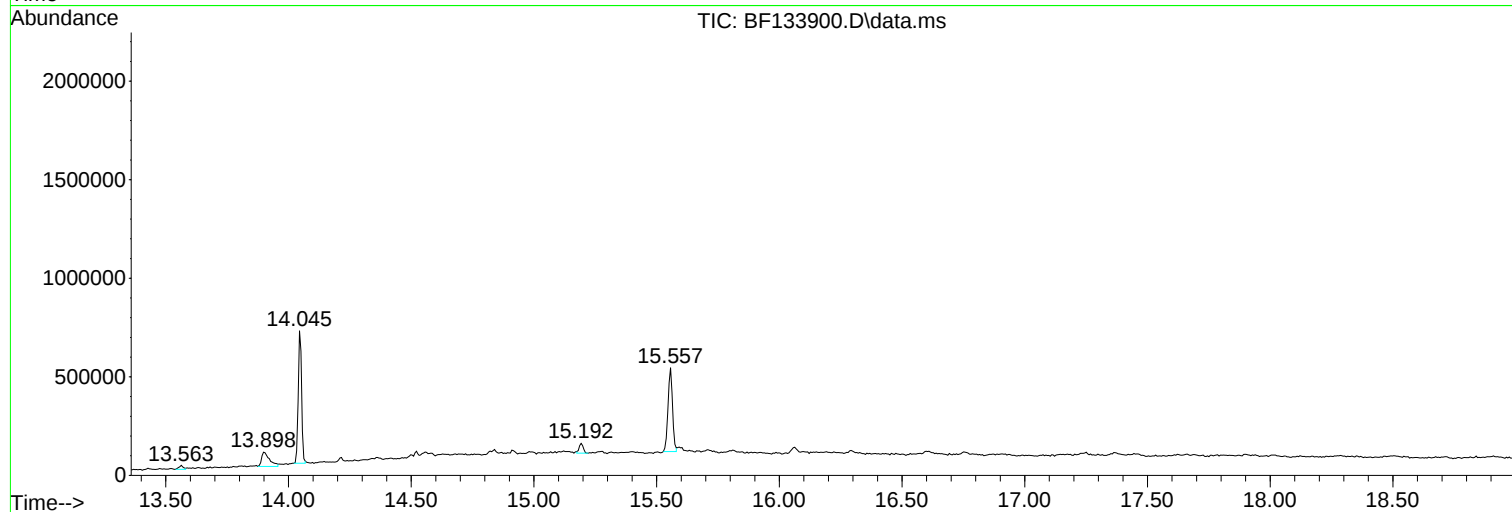
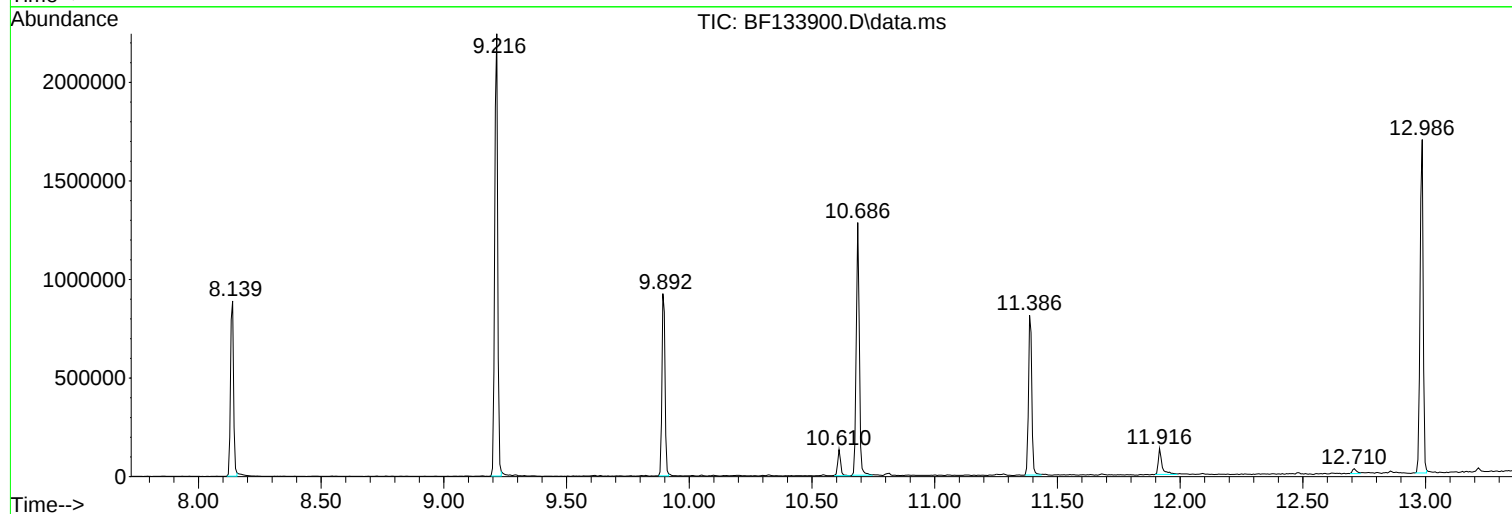
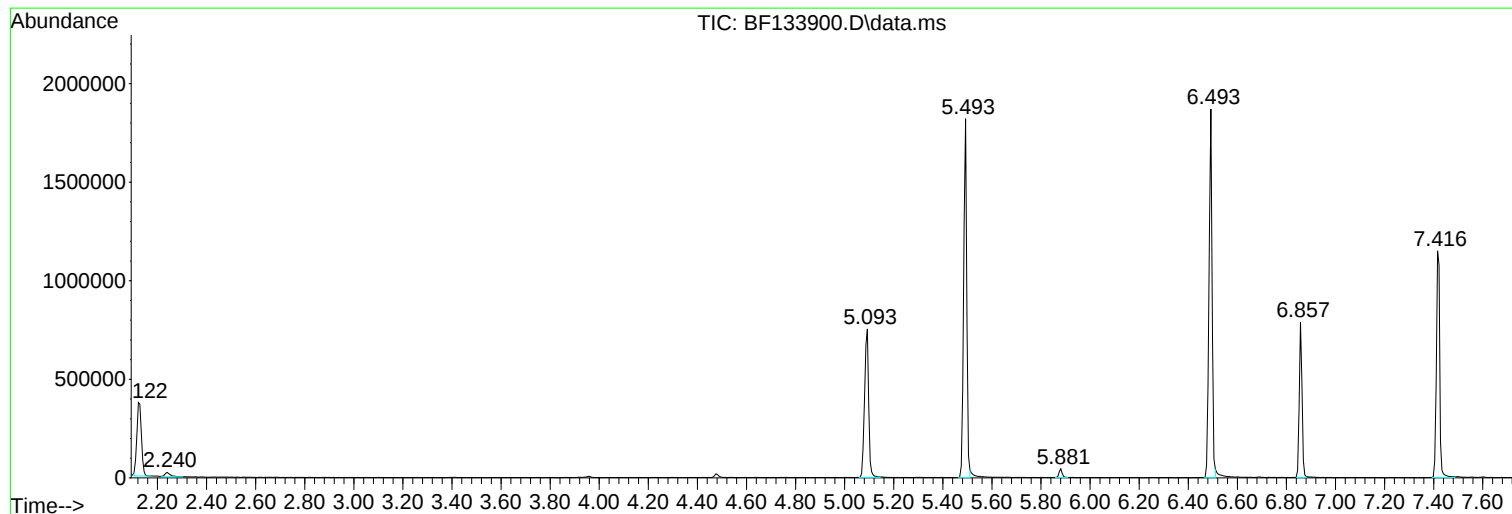
Sum of corrected areas: 14874168

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062223\
Data File : BF133900.D
Acq On : 22 Jun 2023 14:28
Operator : CG\JU
Sample : 03321-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-21

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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\BF062223\
Data File : BF133900.D
Acq On : 22 Jun 2023 14:28
Operator : CG\JU
Sample : 03321-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-21

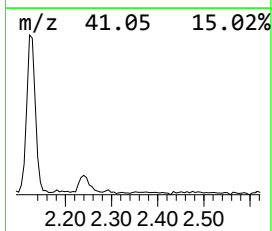
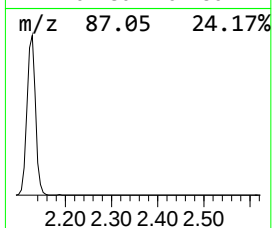
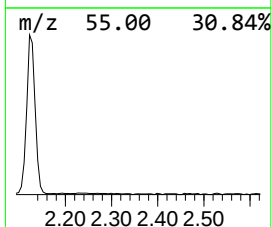
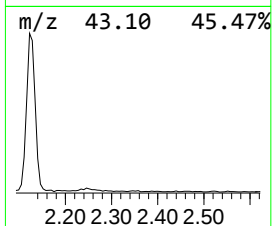
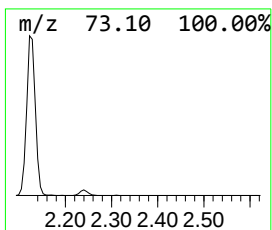
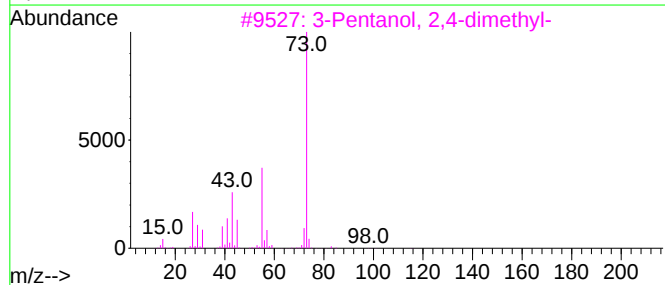
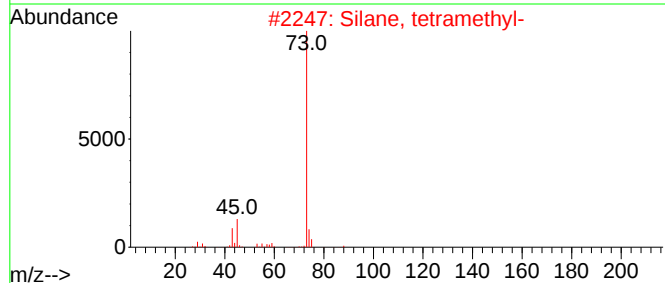
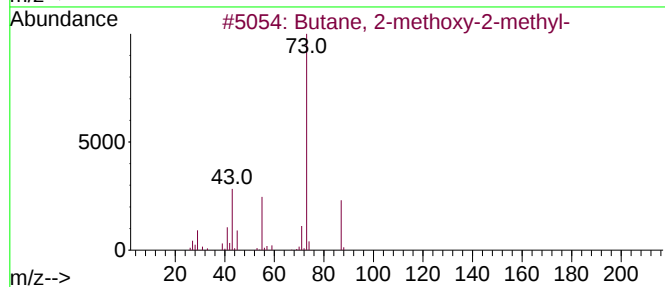
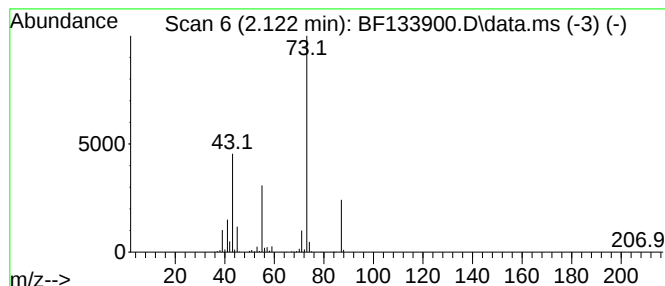
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	15.60 ng	480965	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062223\
Data File : BF133900.D
Acq On : 22 Jun 2023 14:28
Operator : CG\JU
Sample : 03321-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-21

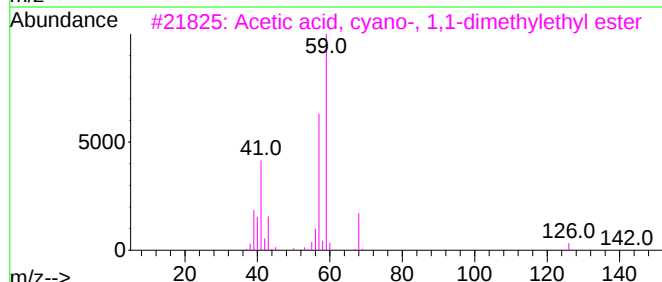
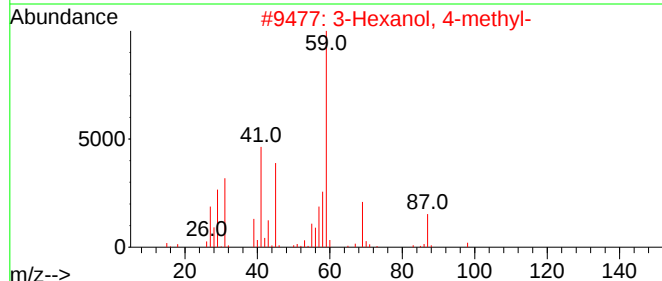
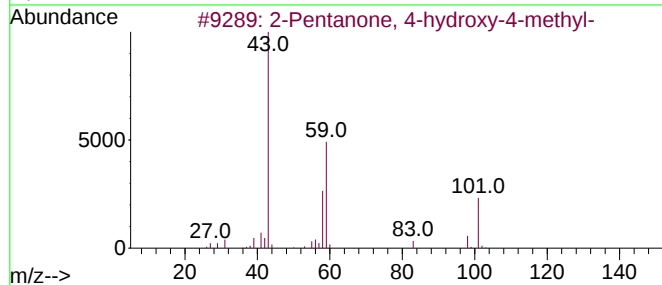
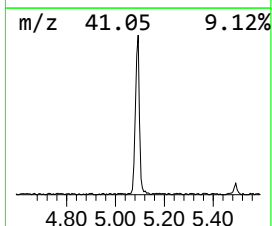
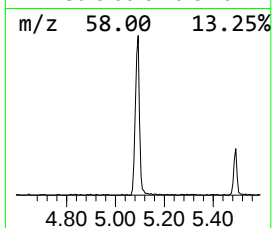
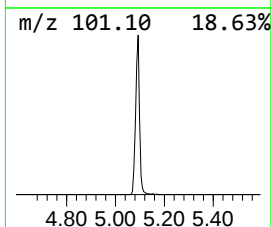
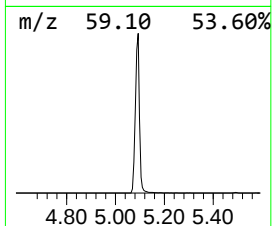
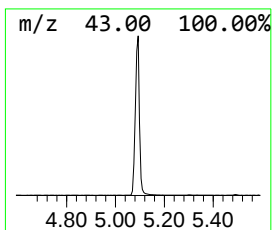
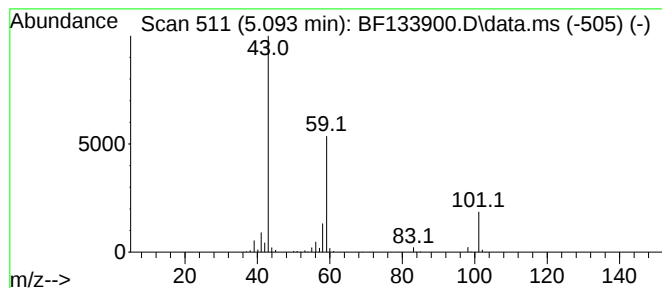
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	28.34 ng	873673	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062223\
Data File : BF133900.D
Acq On : 22 Jun 2023 14:28
Operator : CG\JU
Sample : 03321-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-21

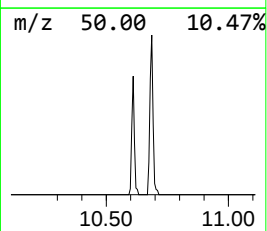
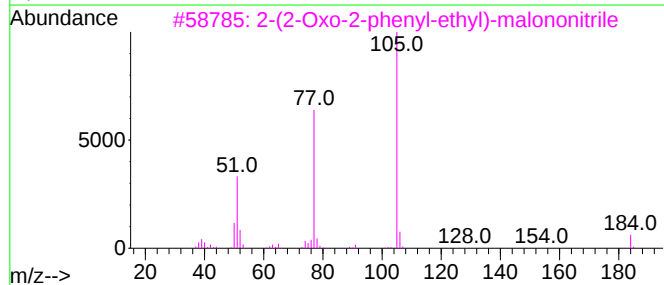
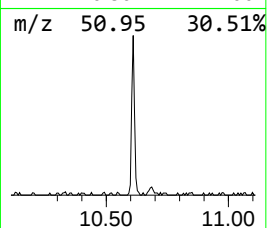
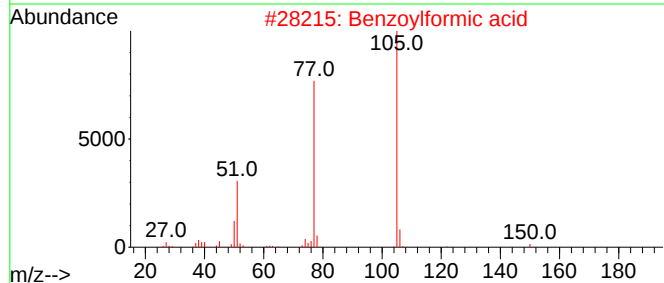
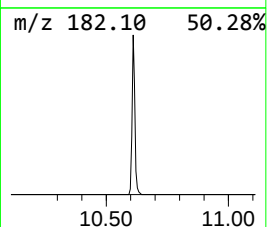
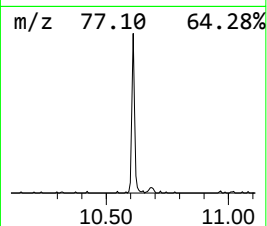
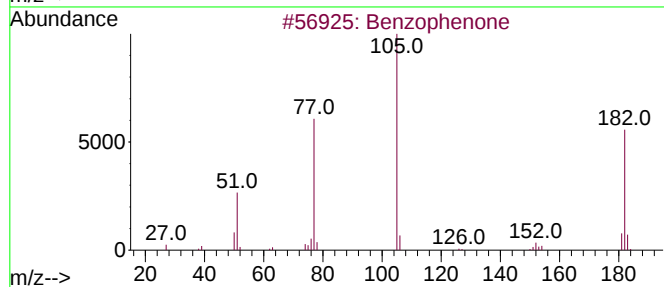
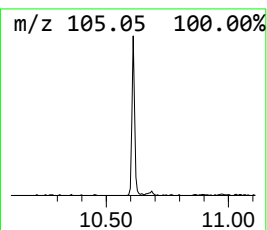
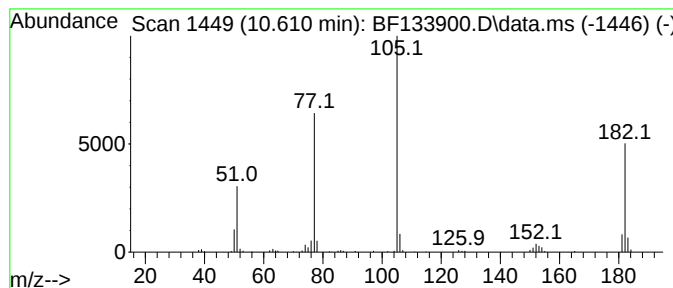
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.610	2.66 ng	107129	Acenaphthene-d10	9.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzoylformic acid	150	C8H6O3	000611-73-4	53
3			2-(2-Oxo-2-phenyl-ethyl)-malononitrile	184	C11H8N2O	1000296-76-9	53
4			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	50
5			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062223\
Data File : BF133900.D
Acq On : 22 Jun 2023 14:28
Operator : CG\JU
Sample : 03321-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-21

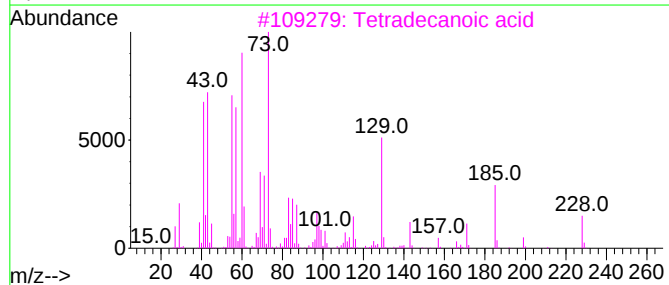
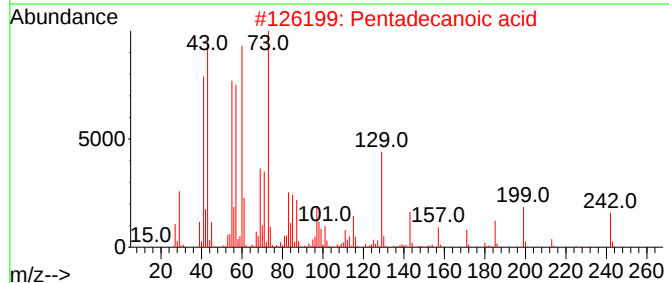
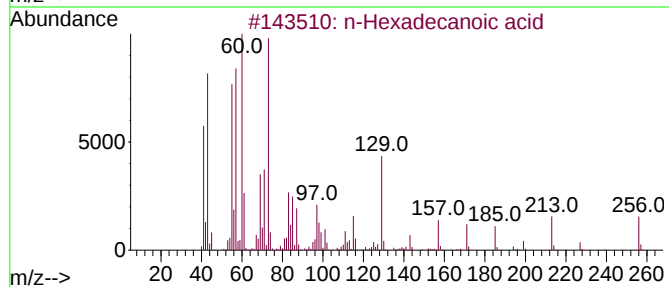
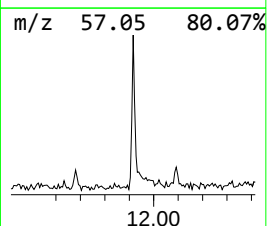
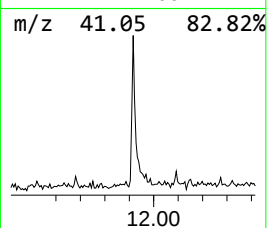
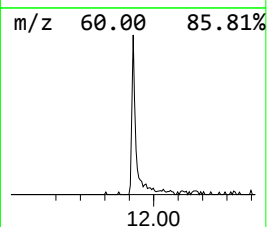
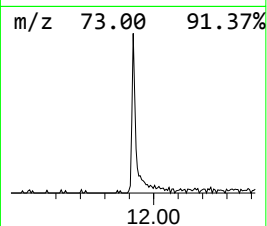
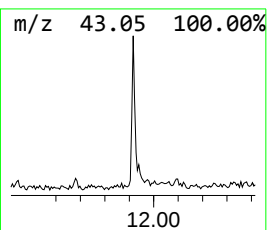
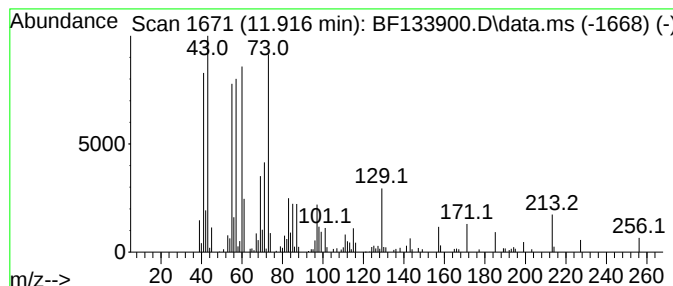
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	3.77 ng	141275	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			Tridecanoic acid	214	C13H26O2	000638-53-9	68
5			Nonanoic acid	158	C9H18O2	000112-05-0	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062223\
Data File : BF133900.D
Acq On : 22 Jun 2023 14:28
Operator : CG\JU
Sample : 03321-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-21

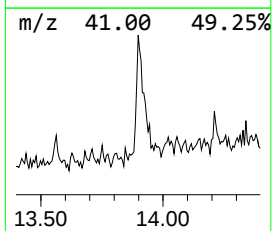
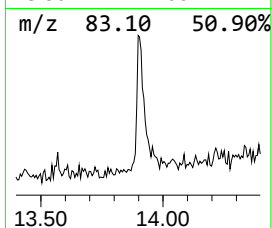
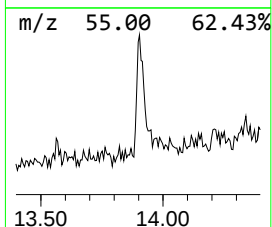
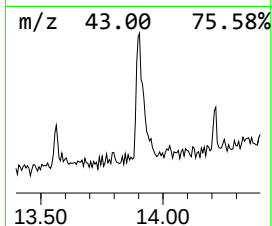
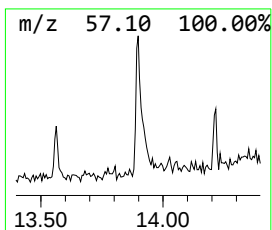
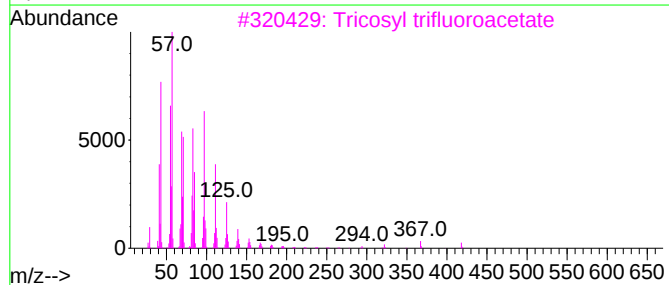
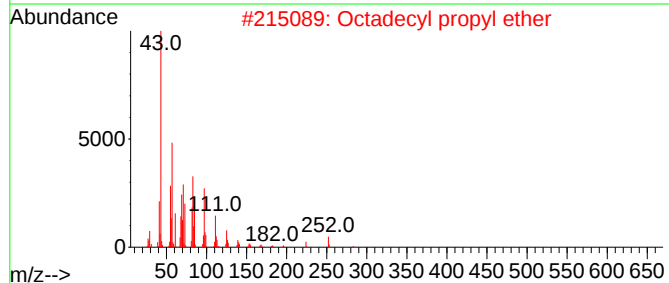
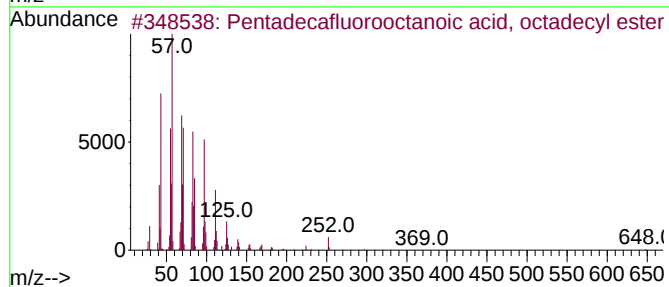
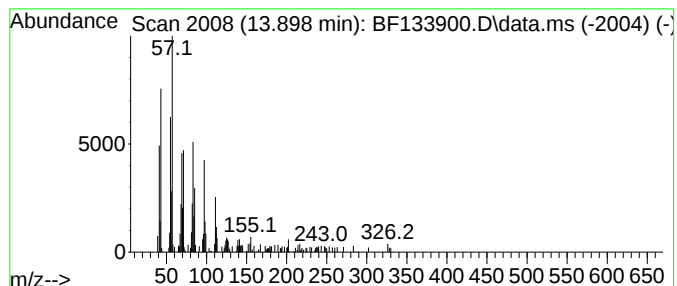
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	5.13 ng	164326	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			Octadecyl propyl ether	312	C21H44O	1000406-28-0	91
3			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
4			Cyclopentane, (4-octyldodecyl)-	350	C25H50	005638-09-5	90
5			Triacontyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062223\
Data File : BF133900.D
Acq On : 22 Jun 2023 14:28
Operator : CG\JU
Sample : 03321-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-21

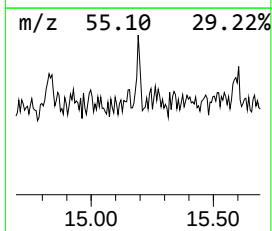
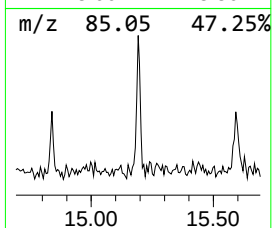
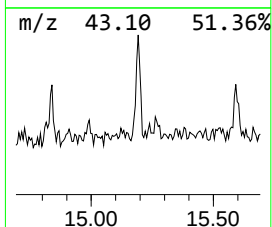
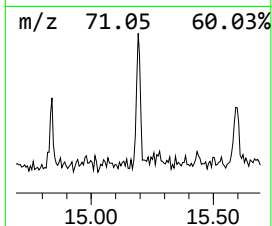
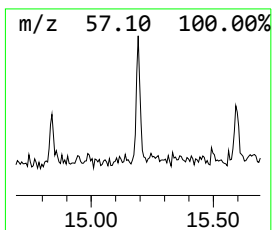
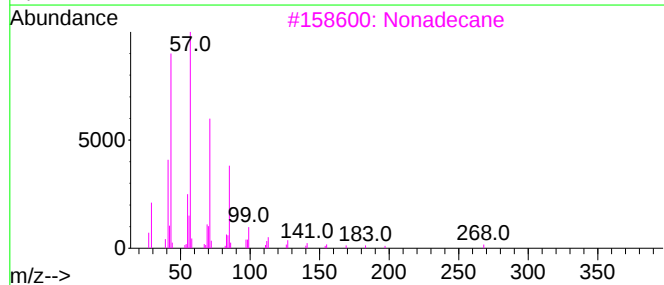
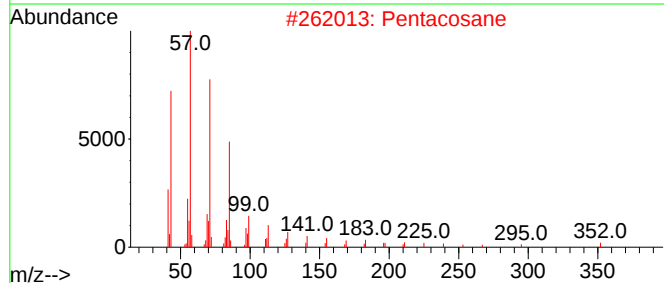
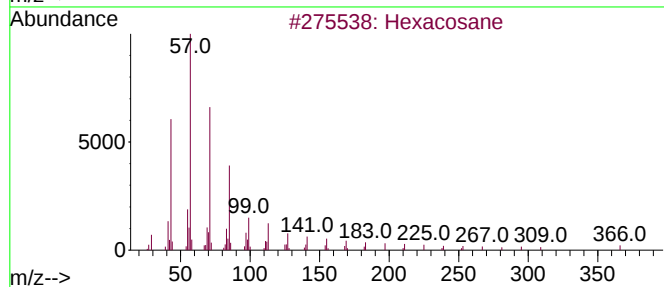
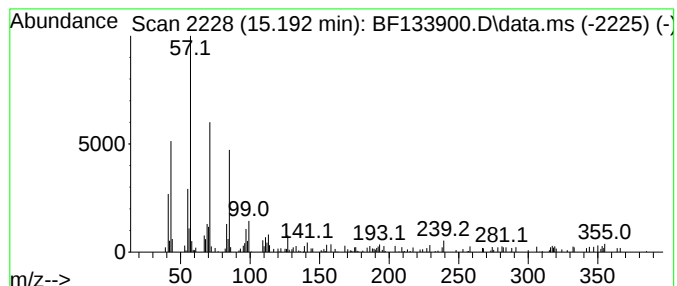
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.192	2.08 ng	56020	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	92
2			Pentacosane	352	C25H52	000629-99-2	91
3			Nonadecane	268	C19H40	000629-92-5	91
4			Eicosane	282	C20H42	000112-95-8	90
5			Heneicosane	296	C21H44	000629-94-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062223\
Data File : BF133900.D
Acq On : 22 Jun 2023 14:28
Operator : CG\JU
Sample : 03321-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-21

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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
Butane, 2-metho...	2.122	15.6	ng	480965	1	6.857	616466	20.0
2-Pentanone, 4-...	5.093	28.3	ng	873673	1	6.857	616466	20.0
Benzophenone	10.610	2.7	ng	107129	3	9.892	806138	20.0
n-Hexadecanoic ...	11.916	3.8	ng	141275	4	11.386	750059	20.0
Pentadecafluoro...	13.898	5.1	ng	164326	5	14.045	640931	20.0
Hexacosane	15.192	2.1	ng	56020	6	15.557	538936	20.0