

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081123\
 Data File : BF134723.D
 Acq On : 11 Aug 2023 09:52
 Operator : CG\JU
 Sample : 03954-16
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-20

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-BF080123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134723.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	11	15	21	rVB5	24358	41611	1.15%	0.160%
2	5.039	498	502	512	rVB	54916	69639	1.92%	0.268%
3	5.434	564	569	572	rBV	3562370	3284931	90.75%	12.637%
4	6.439	734	740	743	rBV	3276811	3318686	91.69%	12.766%
5	6.633	769	773	777	rBV	117754	120187	3.32%	0.462%
6	6.798	798	801	805	rBV	1351505	1042727	28.81%	4.011%
7	7.363	892	897	900	rBV	2368389	2133832	58.95%	8.208%
8	8.075	1015	1018	1022	rBV	1504141	1328083	36.69%	5.109%
9	9.157	1198	1202	1205	rBV	4171178	3619660	100.00%	13.924%
10	9.274	1218	1222	1226	rVB	197477	178835	4.94%	0.688%
11	9.833	1313	1317	1321	rBV	1623254	1328285	36.70%	5.110%
12	10.621	1447	1451	1465	rBV	2246156	1977674	54.64%	7.608%
13	11.321	1566	1570	1573	rBV	1349196	1186700	32.78%	4.565%
14	11.345	1573	1574	1577	rVB	100868	54718	1.51%	0.210%
15	11.857	1657	1661	1671	rBV2	474836	496587	13.72%	1.910%
16	12.433	1753	1759	1761	rBV5	59285	67582	1.87%	0.260%
17	12.533	1773	1776	1780	rBV	170284	160430	4.43%	0.617%
18	12.645	1792	1795	1800	rBV	160051	171200	4.73%	0.659%
19	12.763	1810	1815	1818	rBV	164328	162265	4.48%	0.624%
20	12.915	1837	1841	1844	rBV	3306549	2919327	80.65%	11.230%
21	13.827	1992	1996	2004	rBV2	233475	264935	7.32%	1.019%
22	13.968	2016	2020	2023	rBV	1036629	1008528	27.86%	3.880%
23	14.074	2036	2038	2042	rVB4	52936	46807	1.29%	0.180%
24	14.457	2100	2103	2108	rBV4	68351	115441	3.19%	0.444%
25	14.839	2165	2168	2173	rBV	67334	77149	2.13%	0.297%
26	15.009	2195	2197	2205	rVB	80734	135495	3.74%	0.521%
27	15.439	2266	2270	2278	rVB	574640	684257	18.90%	2.632%

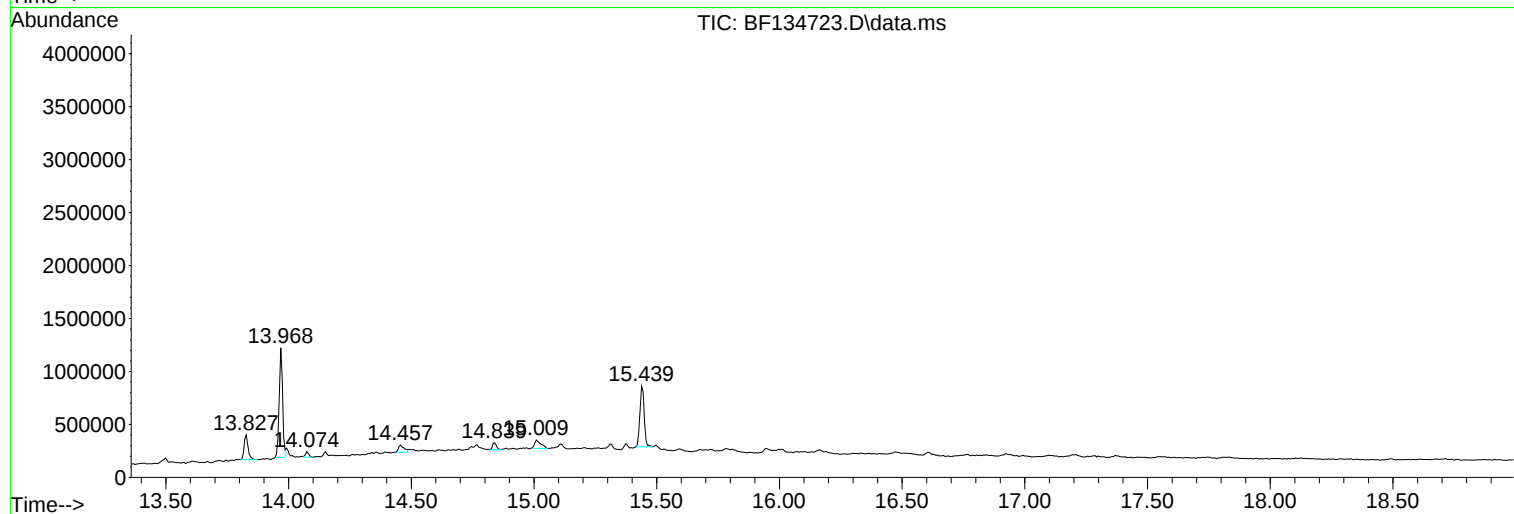
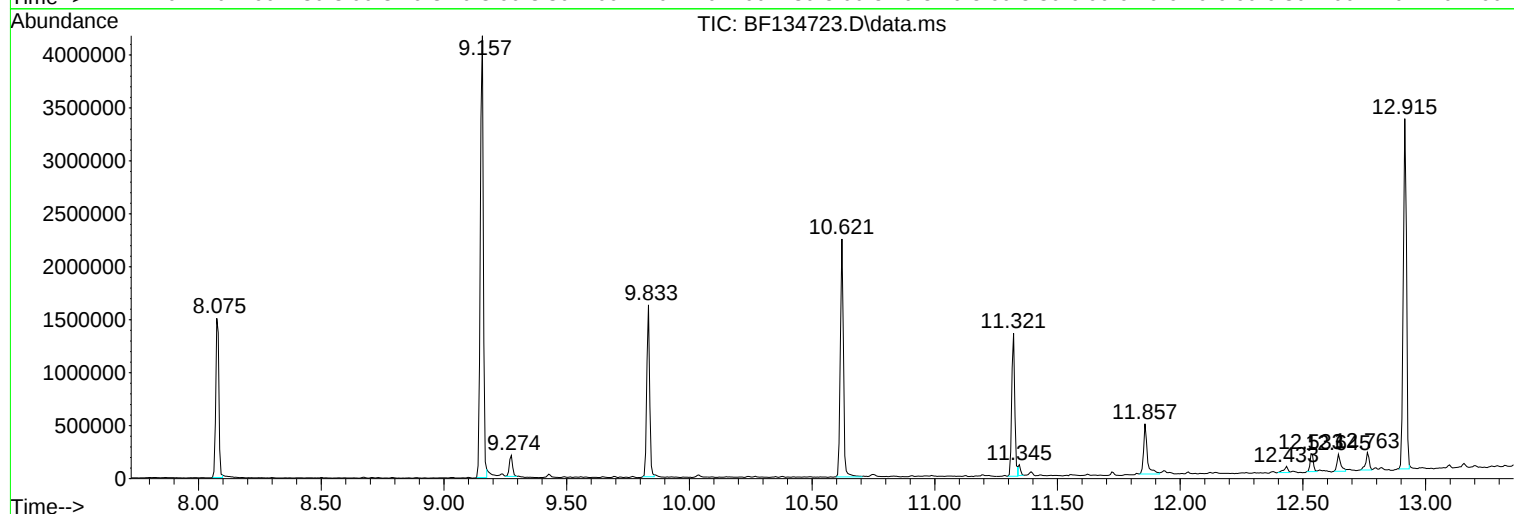
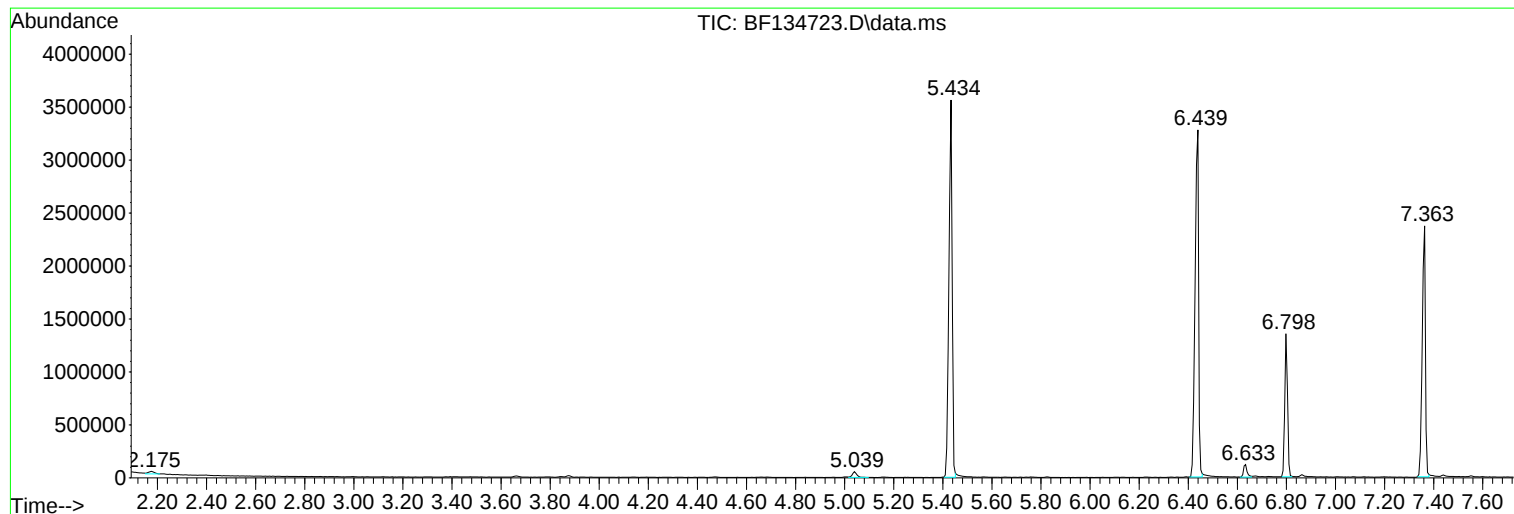
Sum of corrected areas: 25995571

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081123\
Data File : BF134723.D
Acq On : 11 Aug 2023 09:52
Operator : CG\JU
Sample : 03954-16
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-20

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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\BF081123\
Data File : BF134723.D
Acq On : 11 Aug 2023 09:52
Operator : CG\JU
Sample : 03954-16
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-20

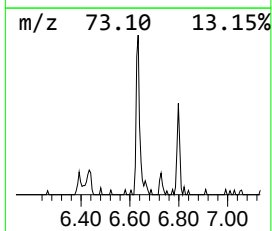
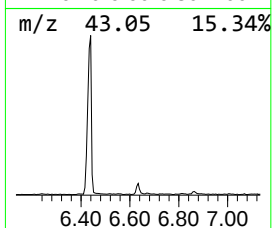
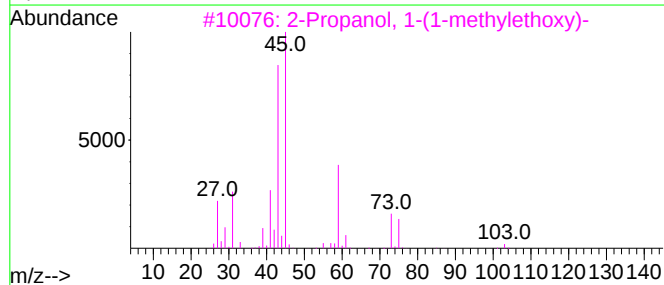
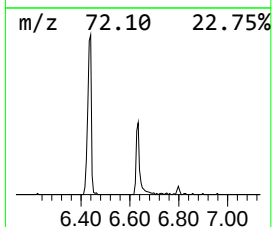
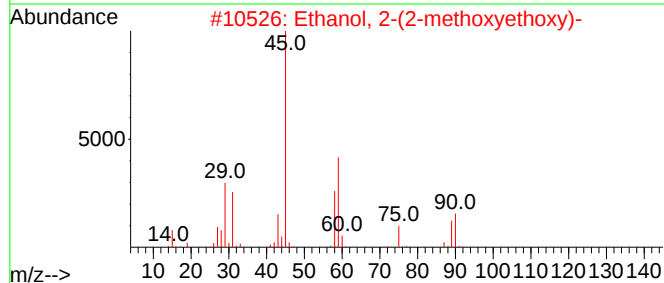
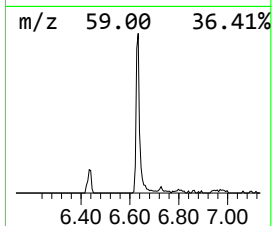
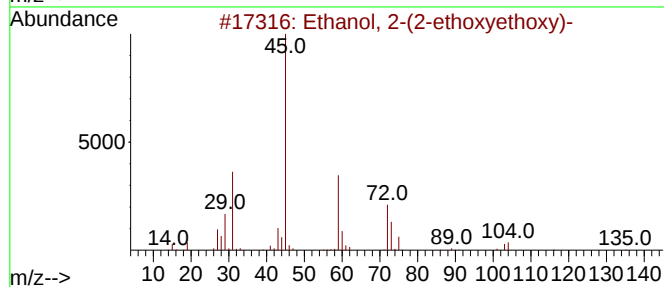
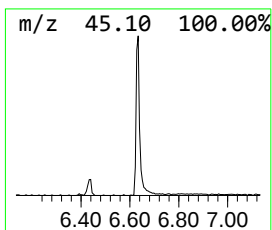
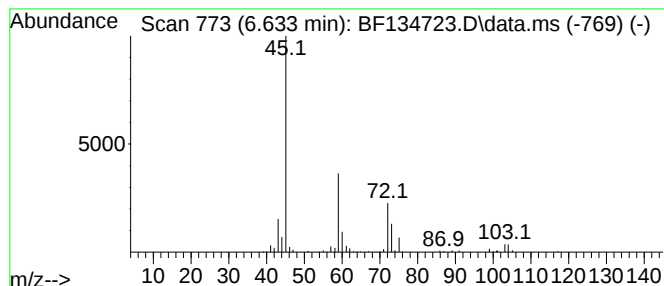
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.633	2.31 ng	120187	1,4-Dichlorobenzene-d4	6.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	42
3			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	42
4			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	40
5			Carbonic acid, dimethyl ester	90	C3H6O3	000616-38-6	36



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081123\
Data File : BF134723.D
Acq On : 11 Aug 2023 09:52
Operator : CG\JU
Sample : 03954-16
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-20

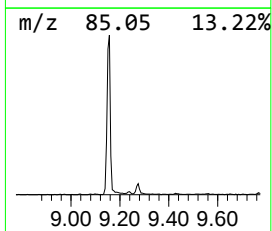
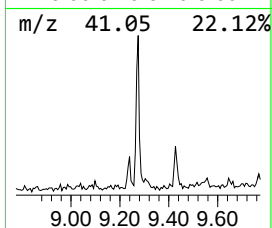
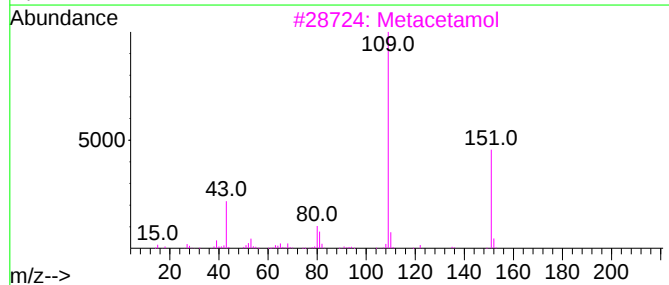
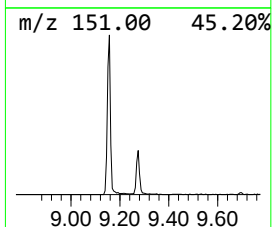
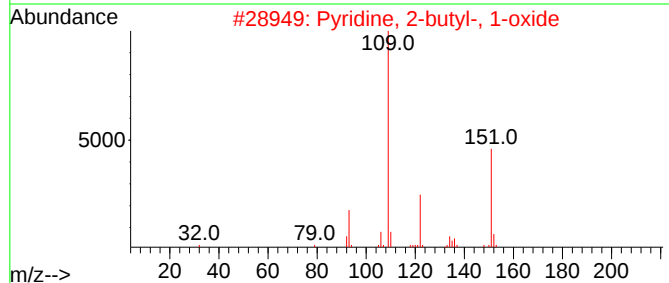
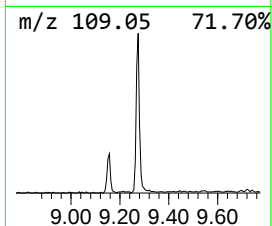
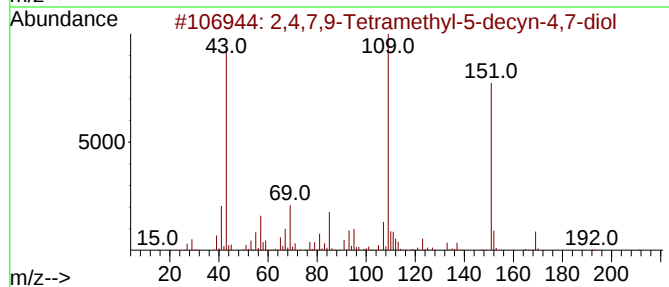
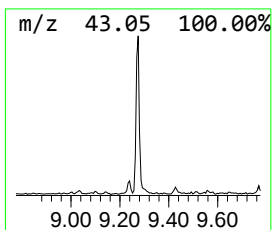
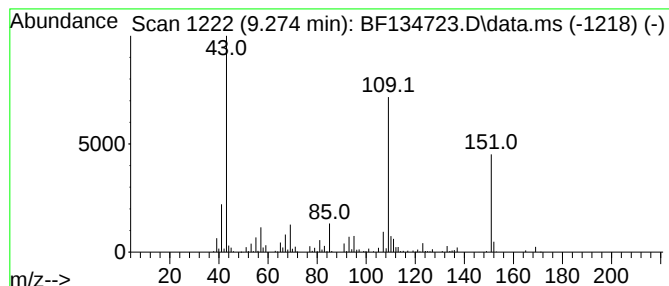
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.274	2.69 ng	178835	Acenaphthene-d10	9.833

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	86		
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53		
3	Metacetamol	151	C8H9NO2	000621-42-1	50		
4	Acetaminophen	151	C8H9NO2	000103-90-2	40		
5	Acetamide, N-(2-hydroxyphenyl)-	151	C8H9NO2	000614-80-2	40		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081123\
Data File : BF134723.D
Acq On : 11 Aug 2023 09:52
Operator : CG\JU
Sample : 03954-16
Misc :
ALS Vial : 5 Sample Multiplier: 1

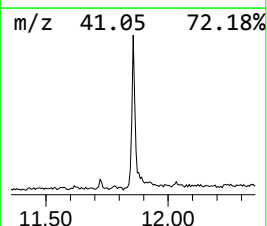
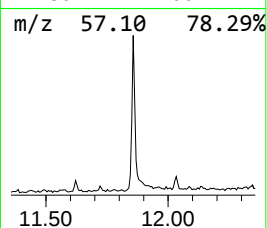
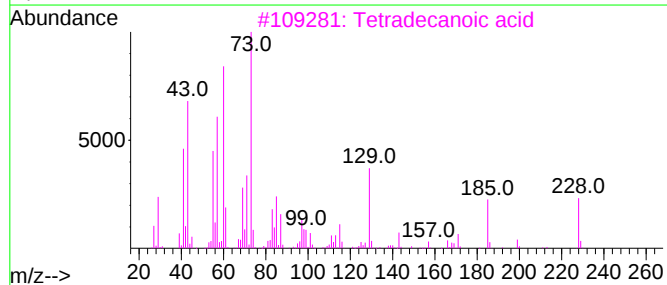
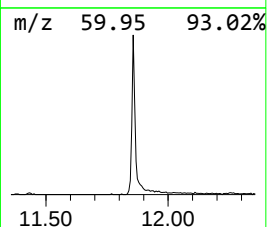
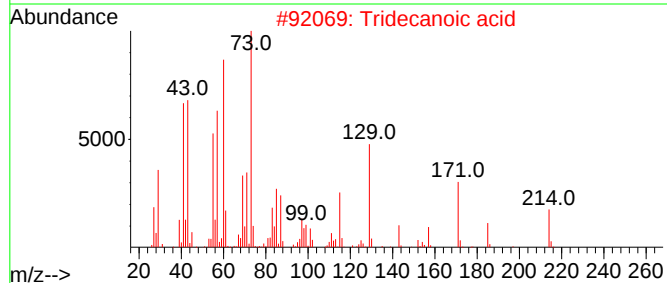
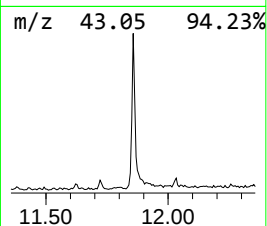
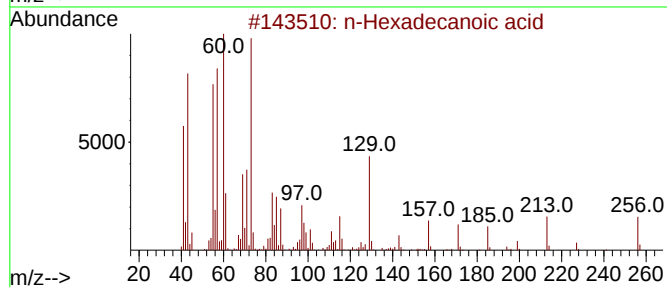
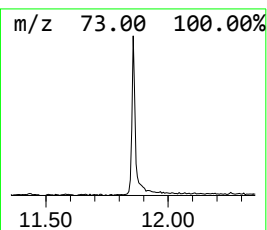
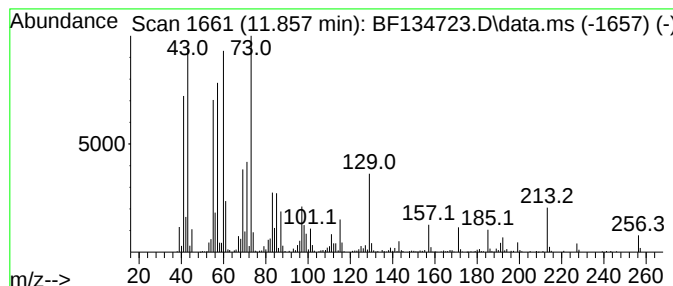
Instrument :
BNA_F
ClientSampleId :
WC-20

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.857	8.37 ng	496587	Phenanthrene-d10	11.321	
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	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081123\
Data File : BF134723.D
Acq On : 11 Aug 2023 09:52
Operator : CG\JU
Sample : 03954-16
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-20

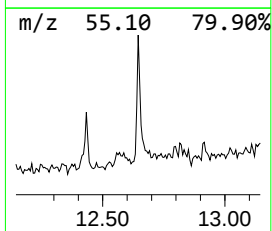
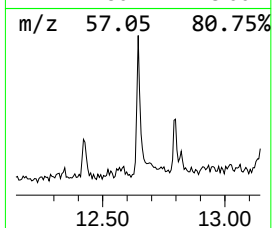
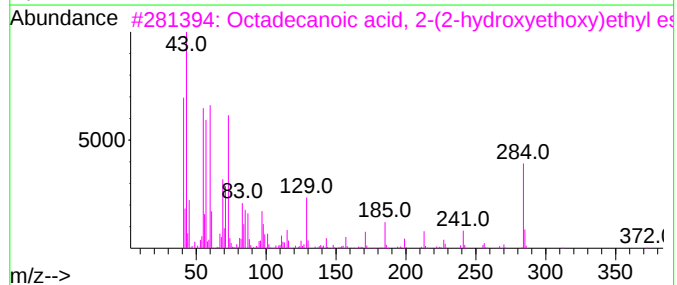
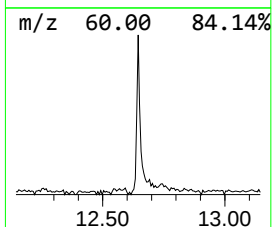
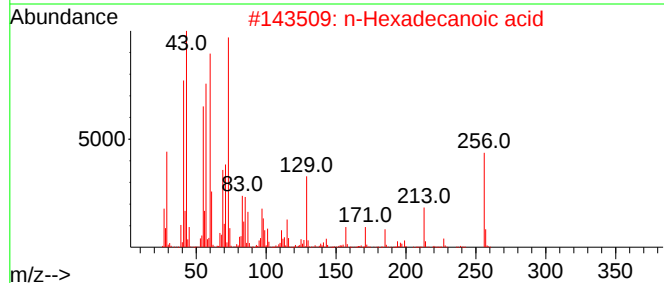
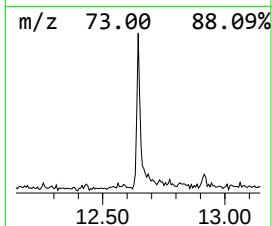
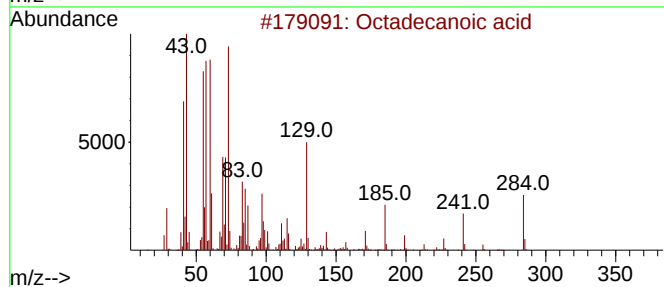
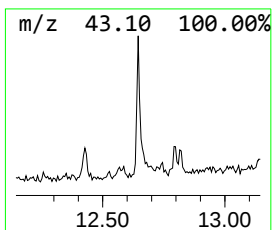
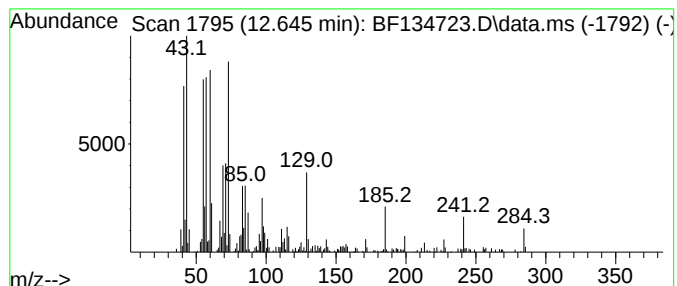
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.645	2.89 ng	171200	Phenanthrene-d10	11.321

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	90
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081123\
Data File : BF134723.D
Acq On : 11 Aug 2023 09:52
Operator : CG\JU
Sample : 03954-16
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-20

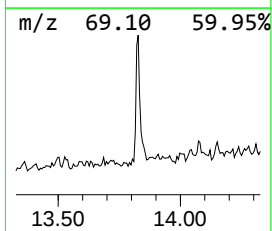
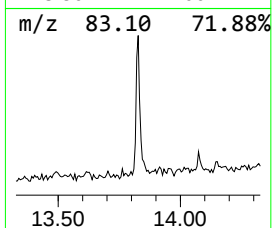
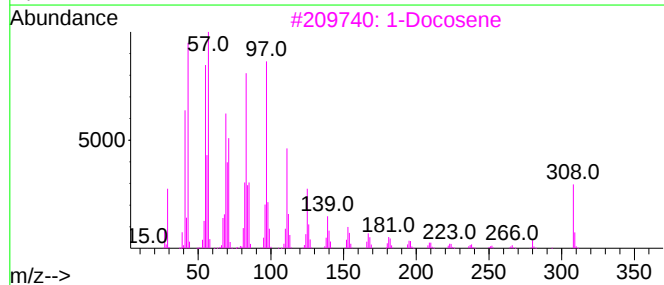
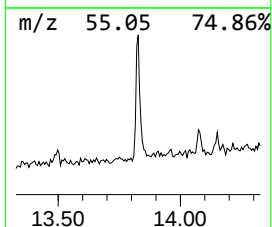
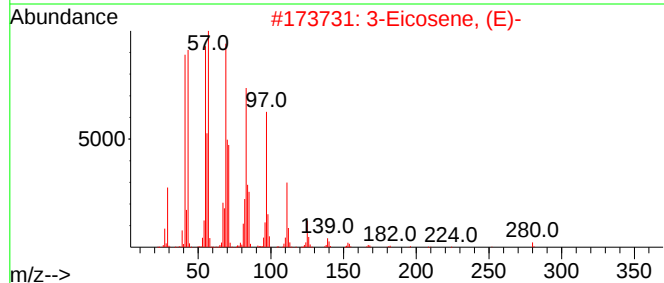
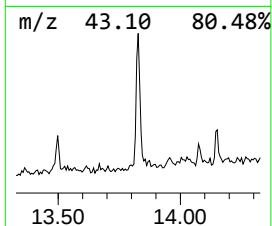
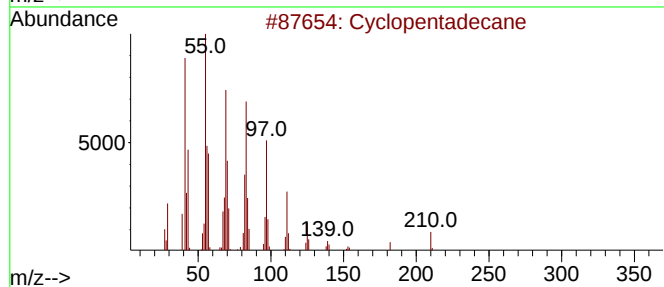
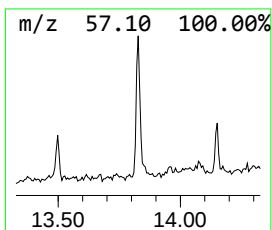
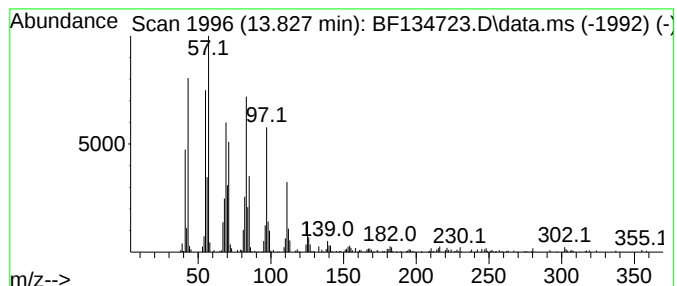
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Cyclopentadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	5.25 ng	264935	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	98
2			3-Eicosene, (E)-	280	C20H40	074685-33-9	96
3			1-Docosene	308	C22H44	001599-67-3	95
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081123\
Data File : BF134723.D
Acq On : 11 Aug 2023 09:52
Operator : CG\JU
Sample : 03954-16
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-20

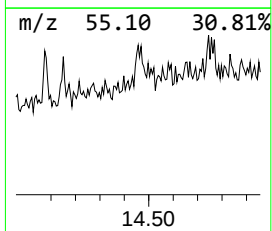
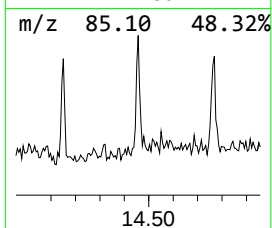
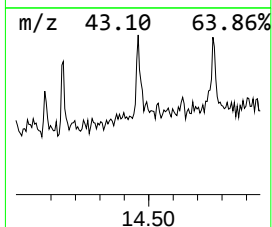
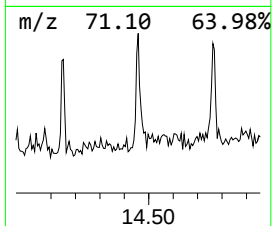
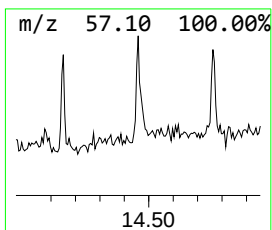
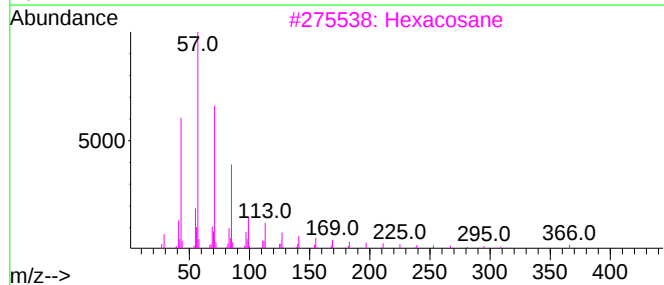
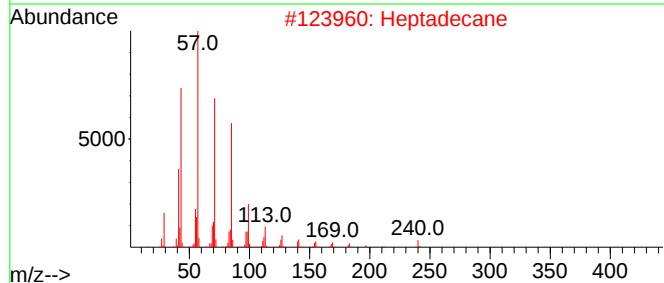
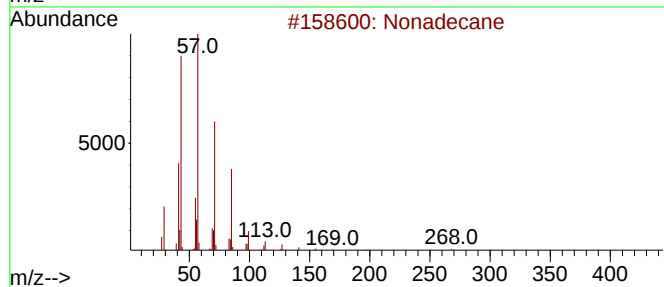
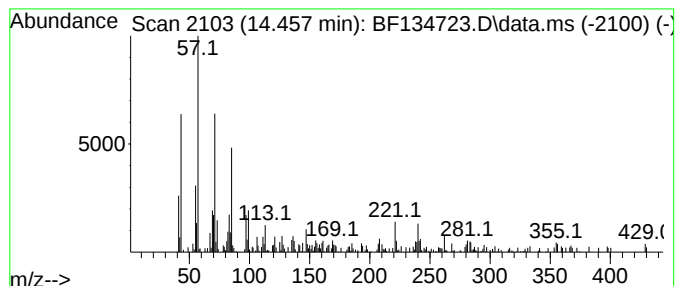
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.457	2.29 ng	115441	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	94
2			Heptadecane	240	C17H36	000629-78-7	90
3			Hexacosane	366	C26H54	000630-01-3	89
4			Hexadecane	226	C16H34	000544-76-3	83
5			Hentriacontane	437	C31H64	000630-04-6	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081123\
Data File : BF134723.D
Acq On : 11 Aug 2023 09:52
Operator : CG\JU
Sample : 03954-16
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-20

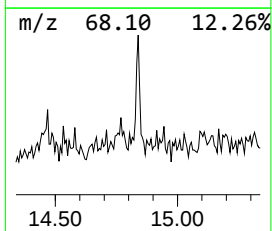
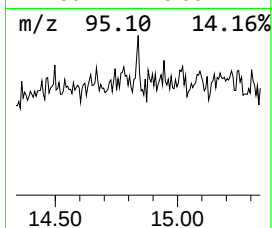
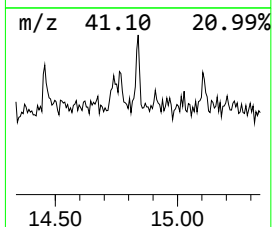
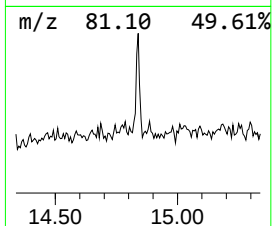
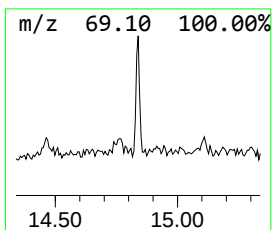
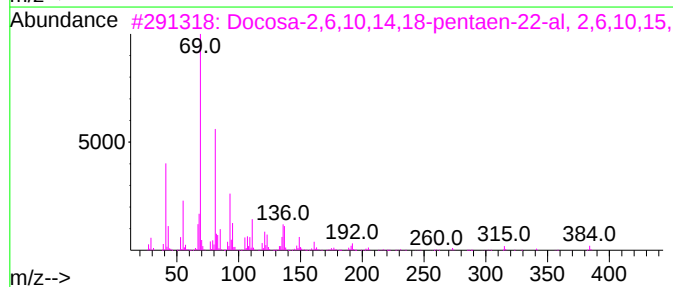
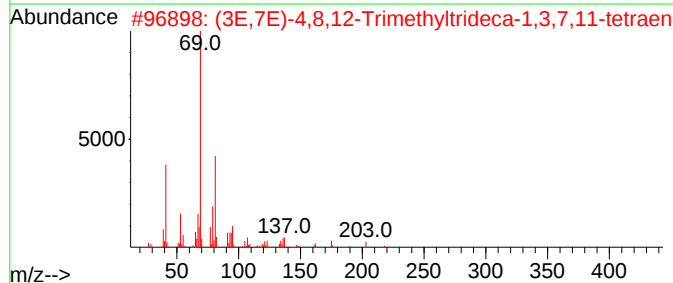
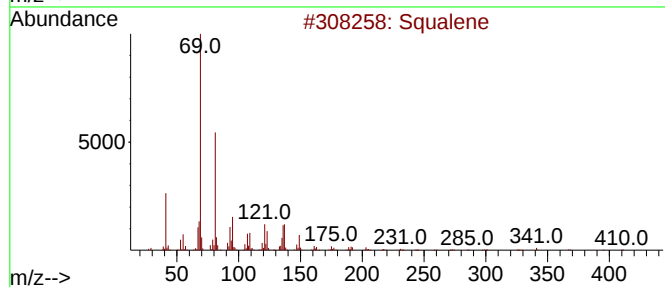
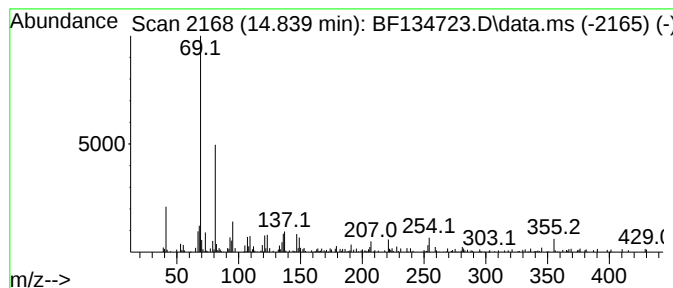
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.839	2.25 ng	77149	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	72
2			(3E,7E)-4,8,12-Trimethyltrideca-...	218	C16H26	062235-06-7	64
3			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	64
4			trans-Farnesol	222	C15H26O	000106-28-5	62
5			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081123\
Data File : BF134723.D
Acq On : 11 Aug 2023 09:52
Operator : CG\JU
Sample : 03954-16
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-20

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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
Ethanol, 2-(2-e...	6.633	2.3	ng	120187	1	6.798	1042730	20.0
2,4,7,9-Tetrame...	9.274	2.7	ng	178835	3	9.833	1328290	20.0
n-Hexadecanoic ...	11.857	8.4	ng	496587	4	11.321	1186700	20.0
Octadecanoic acid	12.645	2.9	ng	171200	4	11.321	1186700	20.0
Cyclopentadecane	13.827	5.3	ng	264935	5	13.968	1008530	20.0
Nonadecane	14.457	2.3	ng	115441	5	13.968	1008530	20.0
Squalene	14.839	2.3	ng	77149	6	15.439	684257	20.0