

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011625\
 Data File : BF141186.D
 Acq On : 16 Jan 2025 15:39
 Operator : RC/JU
 Sample : Q1094-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 72-11938

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-BF011025.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141186.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	6	13	rVB	1564787	2200582	8.58%	3.015%
2	5.045	492	502	512	rVB	235048	424938	1.66%	0.582%
3	5.439	557	569	574	rBV	3416102	4809225	18.75%	6.590%
4	6.445	730	740	746	rBV	3265810	4860315	18.95%	6.660%
5	6.810	797	802	809	rBV	746265	955202	3.72%	1.309%
6	7.375	890	898	903	rBV	2302874	3300052	12.87%	4.522%
7	8.092	1014	1020	1029	rBV2	930846	1537499	5.99%	2.107%
8	9.175	1197	1204	1209	rBV	4278996	5752515	22.43%	7.882%
9	9.851	1311	1319	1323	rBV	1055672	1399354	5.46%	1.917%
10	10.057	1348	1354	1359	rBV	242755	342336	1.33%	0.469%
11	10.569	1436	1441	1446	rVB	417105	550267	2.15%	0.754%
12	10.639	1447	1453	1458	rBV	2154714	2811219	10.96%	3.852%
13	11.339	1567	1572	1574	rBV	848420	1141860	4.45%	1.565%
14	11.363	1574	1576	1580	rVV	623121	668081	2.60%	0.915%
15	11.880	1657	1664	1672	rBV2	2096229	3693867	14.40%	5.061%
16	11.957	1673	1677	1678	rBV	185613	257878	1.01%	0.353%
17	12.557	1775	1779	1781	rBV	834655	1185017	4.62%	1.624%
18	12.668	1794	1798	1802	rVB	1636462	2143168	8.36%	2.937%
19	12.927	1838	1842	1850	rVB	3084344	4530811	17.67%	6.208%
20	13.839	1993	1997	2005	rVB3	233606	407830	1.59%	0.559%
21	13.980	2015	2021	2032	rVB3	921953	1966347	7.67%	2.694%
22	15.021	2194	2198	2207	rVB	349803	760392	2.96%	1.042%
23	15.109	2210	2213	2218	rBV2	184597	301587	1.18%	0.413%
24	15.321	2246	2249	2254	rVB	193870	280841	1.09%	0.385%
25	15.380	2256	2259	2265	rVB	207616	289217	1.13%	0.396%
26	15.445	2266	2270	2275	rBV	488424	762586	2.97%	1.045%
27	15.909	2322	2349	2373	rVB2	3831792	25647829	100.00%	35.143%

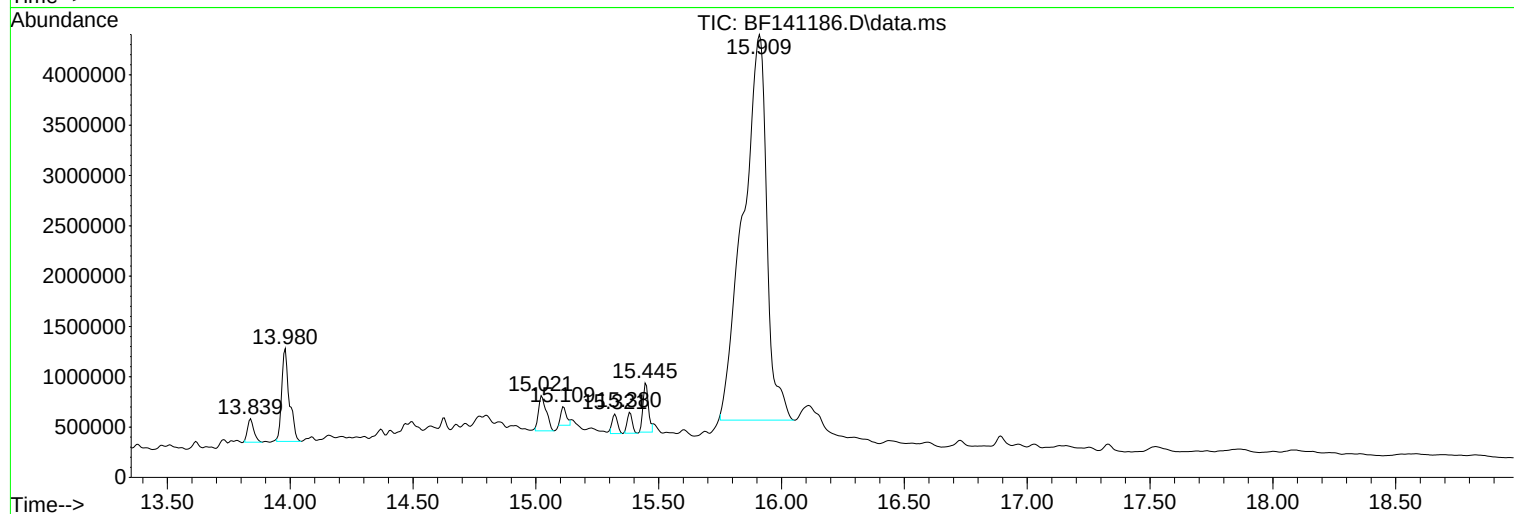
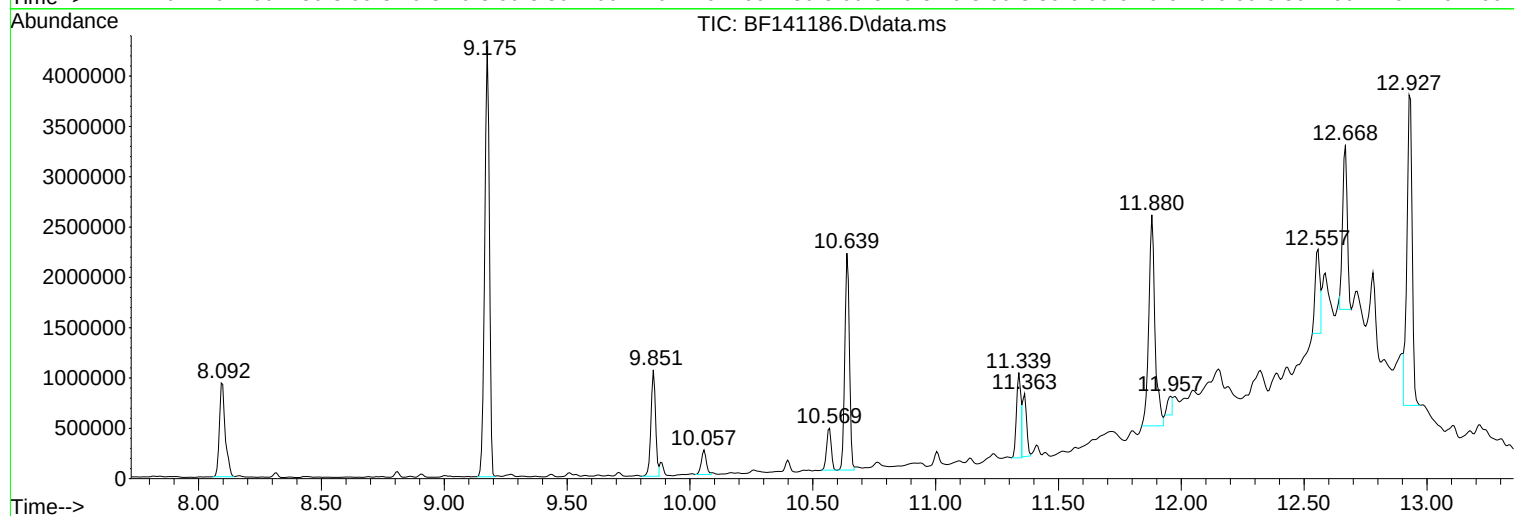
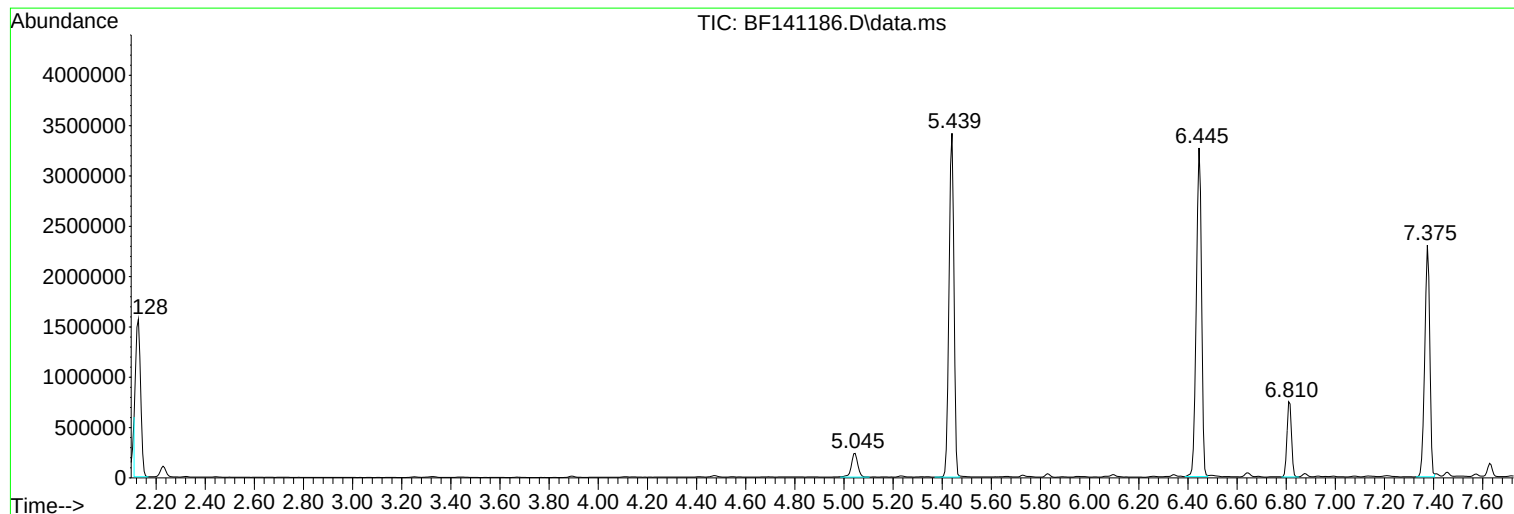
Sum of corrected areas: 72980815

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011625\
Data File : BF141186.D
Acq On : 16 Jan 2025 15:39
Operator : RC/JU
Sample : Q1094-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11938

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.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\BF011625\
Data File : BF141186.D
Acq On : 16 Jan 2025 15:39
Operator : RC/JU
Sample : Q1094-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11938

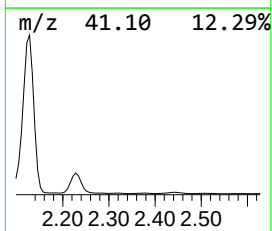
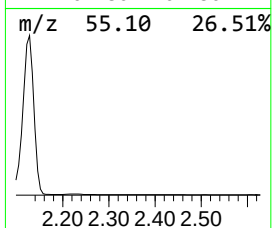
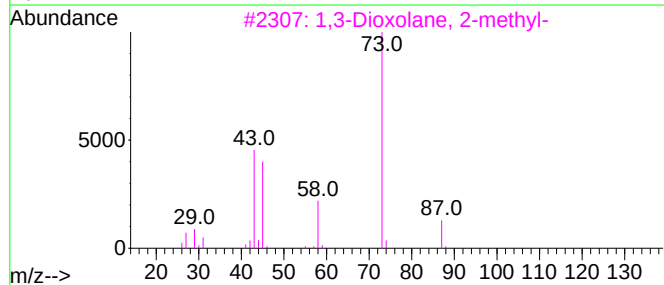
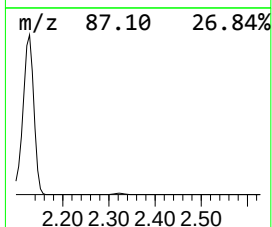
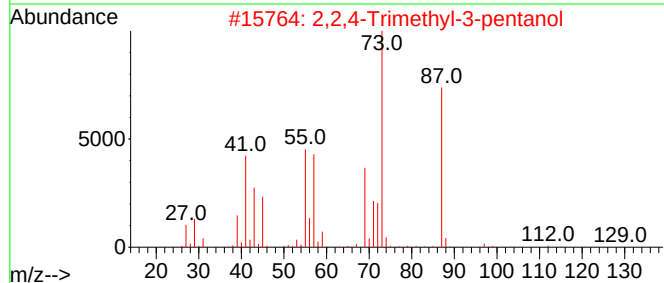
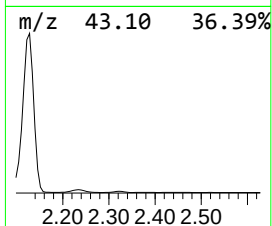
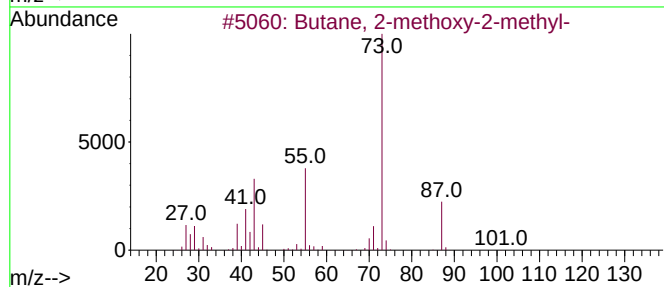
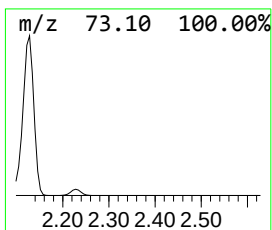
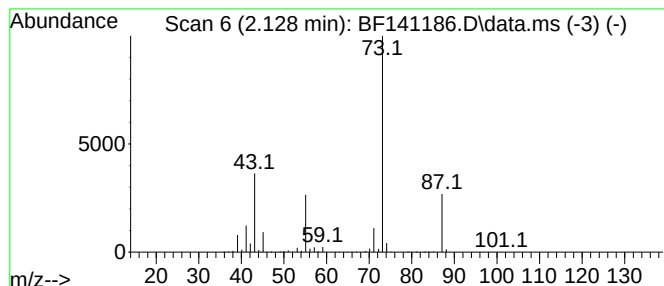
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.128	46.08 ng	2200580	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011625\
Data File : BF141186.D
Acq On : 16 Jan 2025 15:39
Operator : RC/JU
Sample : Q1094-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11938

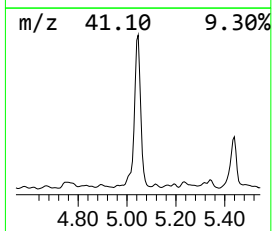
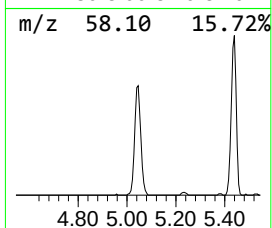
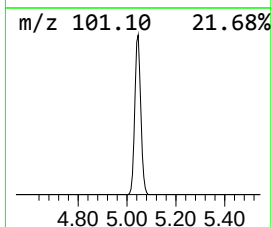
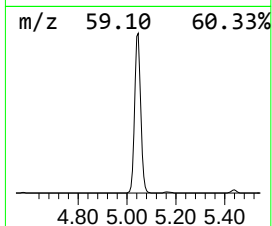
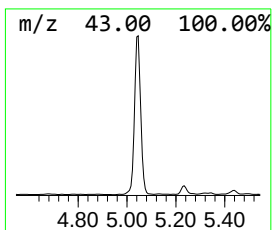
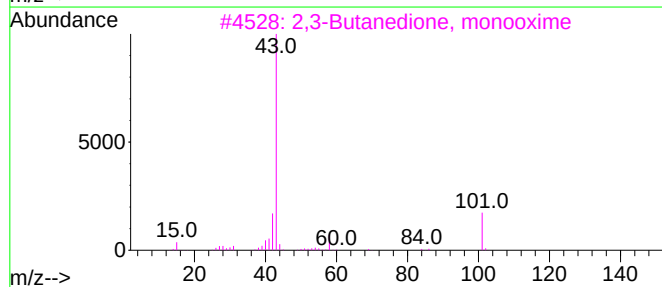
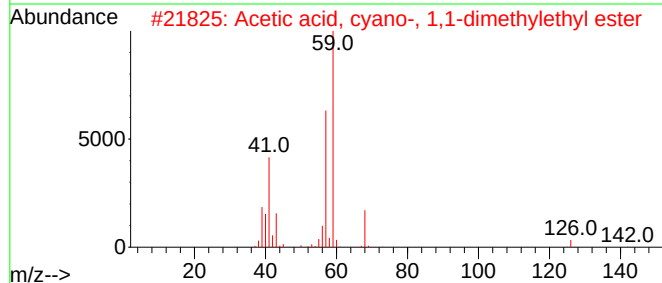
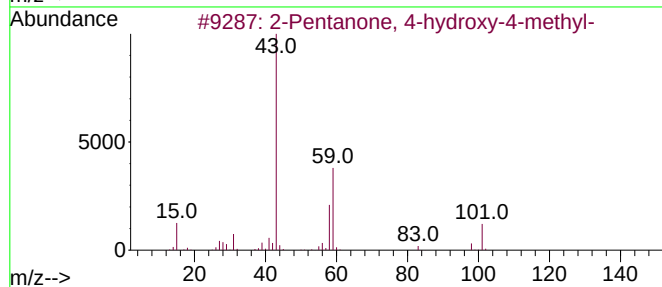
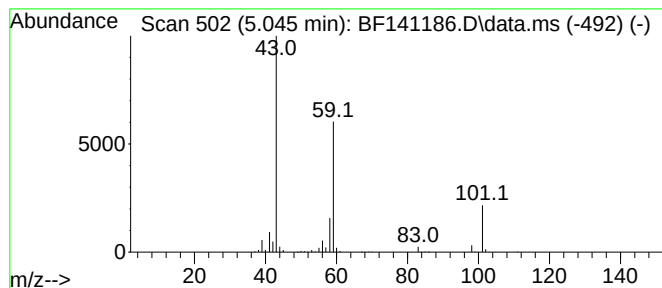
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.045	8.90 ng	424938	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011625\
Data File : BF141186.D
Acq On : 16 Jan 2025 15:39
Operator : RC/JU
Sample : Q1094-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11938

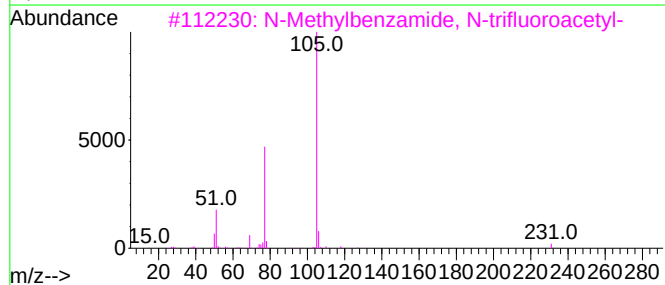
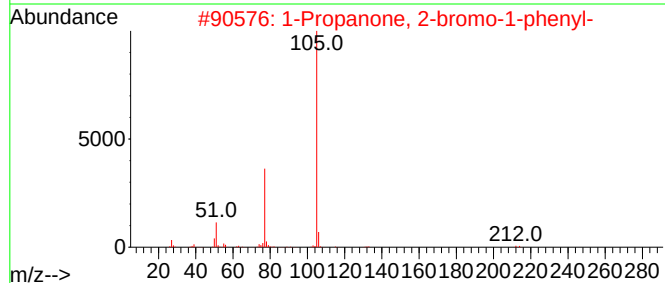
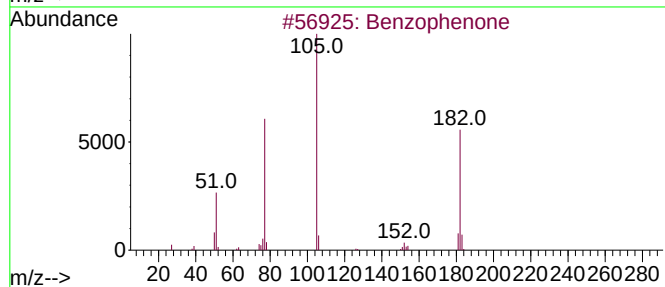
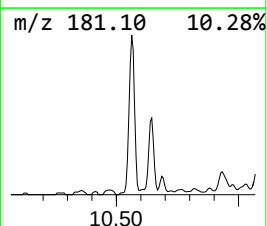
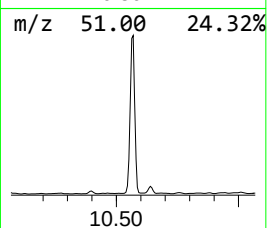
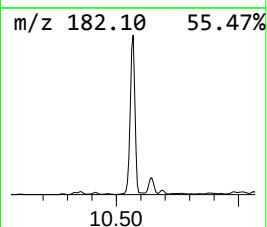
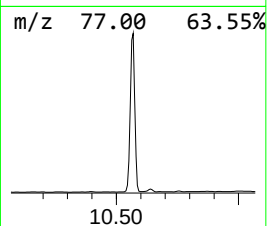
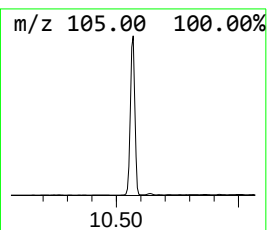
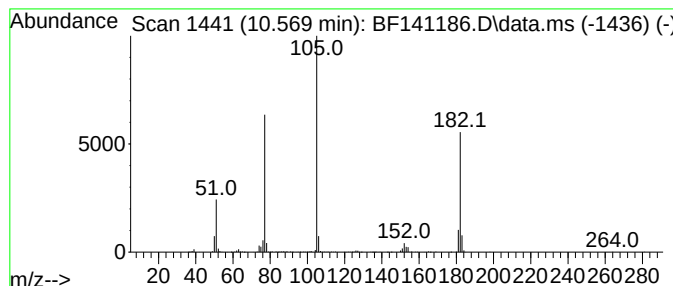
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.569	7.86 ng	550267	Acenaphthene-d10	9.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
3			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47
4			2-Chloro-1-phenyl-1-propanone	168	C9H9ClO	006084-17-9	47
5			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011625\
Data File : BF141186.D
Acq On : 16 Jan 2025 15:39
Operator : RC/JU
Sample : Q1094-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11938

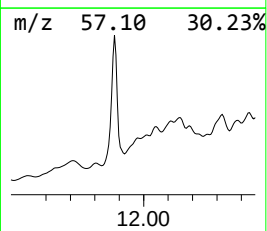
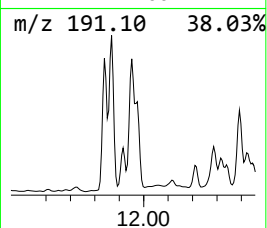
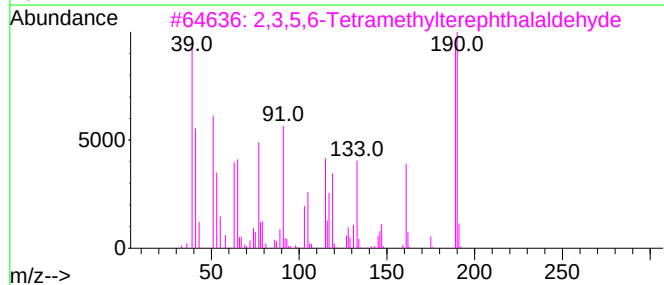
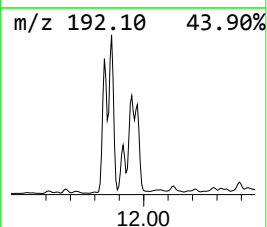
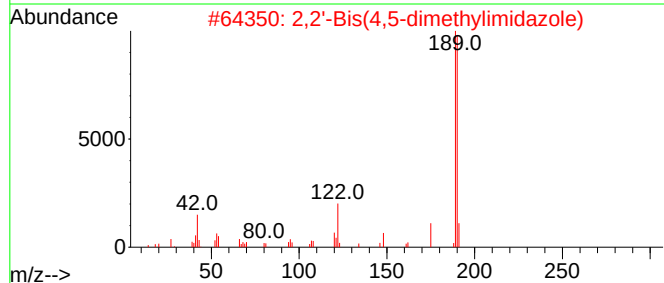
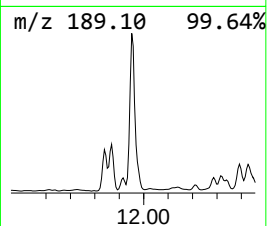
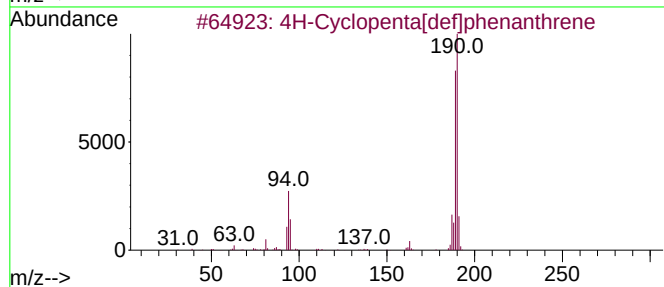
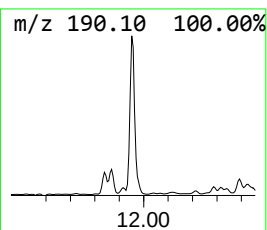
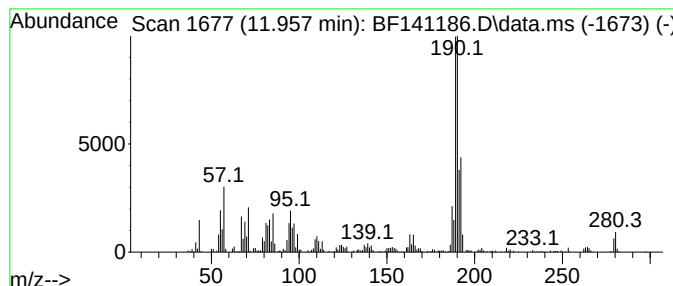
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	4.52 ng	257878	Phenanthrene-d10	11.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	68
2			2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	47
3			2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	46
4			Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	38
5			Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011625\
Data File : BF141186.D
Acq On : 16 Jan 2025 15:39
Operator : RC/JU
Sample : Q1094-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11938

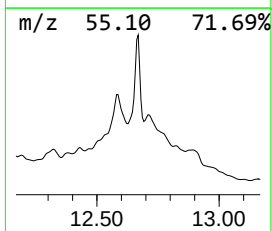
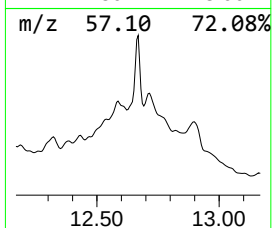
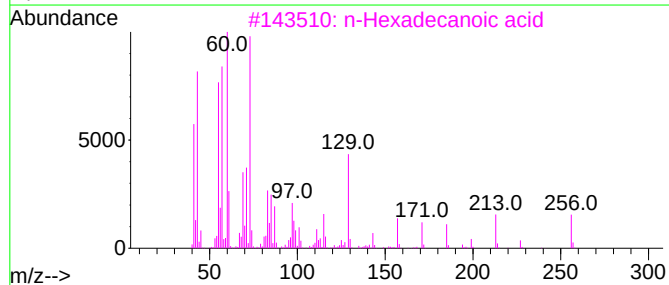
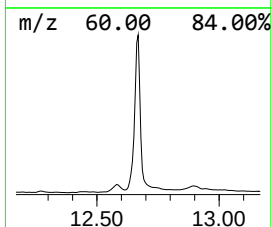
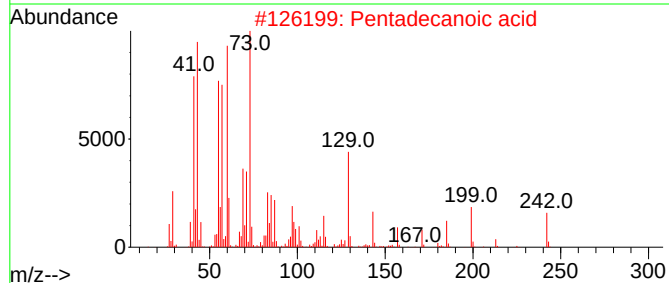
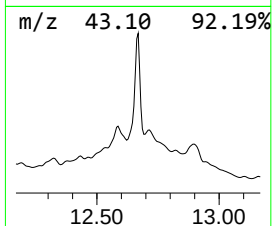
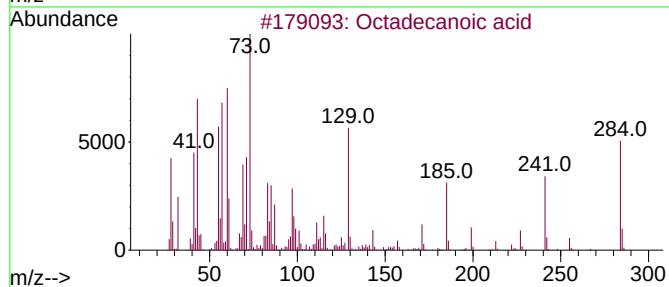
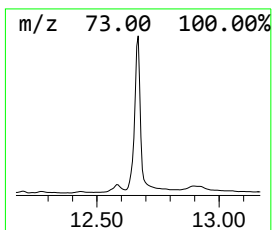
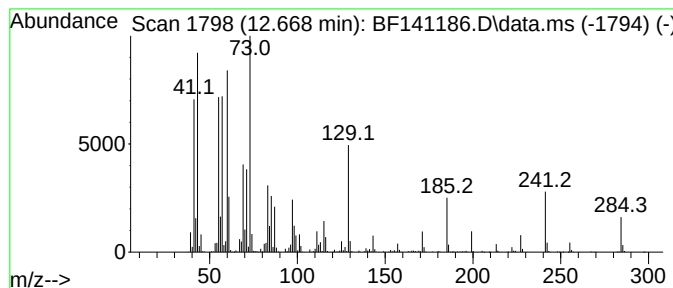
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.668	21.80 ng	2143170	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Oxalic acid, allyl tetradecyl ester	326	C19H34O4	1000309-24-2	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011625\
Data File : BF141186.D
Acq On : 16 Jan 2025 15:39
Operator : RC/JU
Sample : Q1094-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

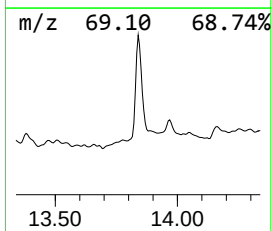
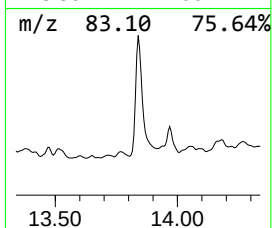
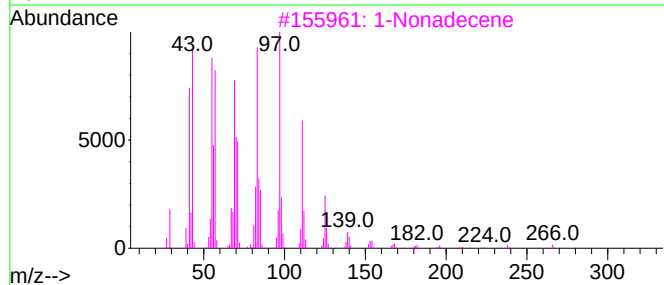
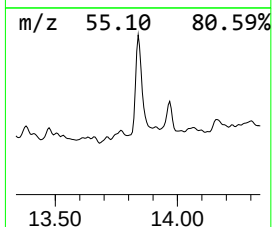
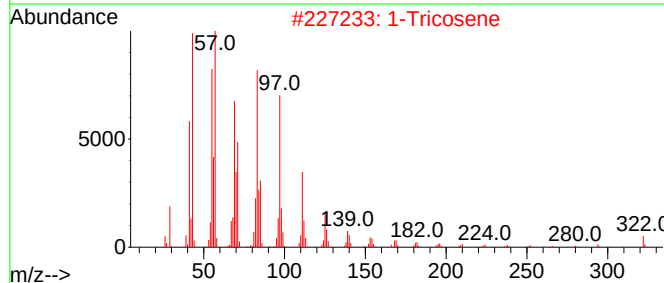
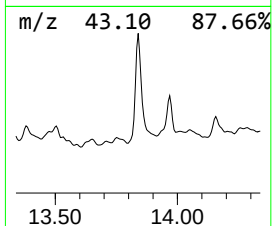
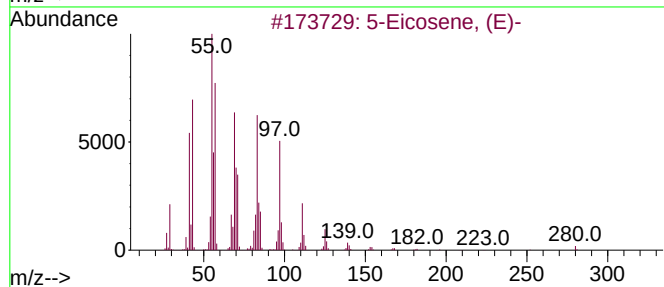
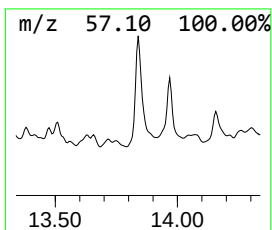
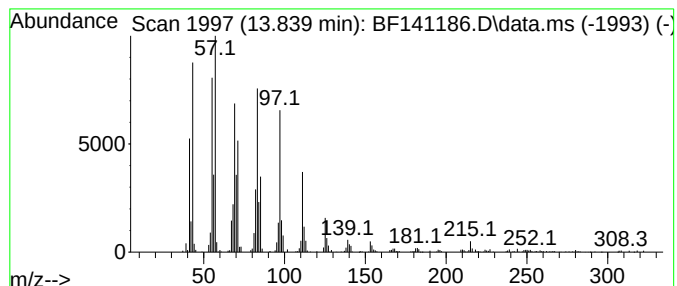
Instrument :
BNA_F
ClientSampleId :
72-11938

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5-Eicosene, (E)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.839	4.15 ng	407830	Chrysene-d12		13.980	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	98
2	1-Tricosene		322	C23H46	018835-32-0	97
3	1-Nonadecene		266	C19H38	018435-45-5	96
4	1-Octadecene		252	C18H36	000112-88-9	96
5	9-Tricosene, (Z)-		322	C23H46	027519-02-4	96



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011625\
Data File : BF141186.D
Acq On : 16 Jan 2025 15:39
Operator : RC/JU
Sample : Q1094-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11938

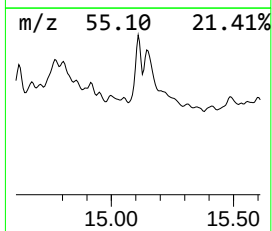
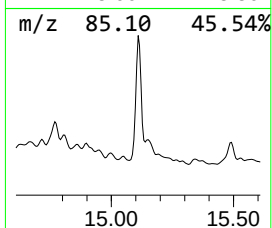
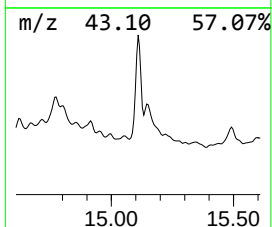
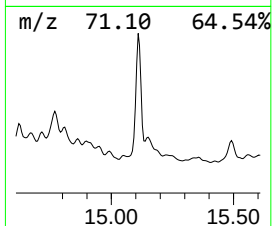
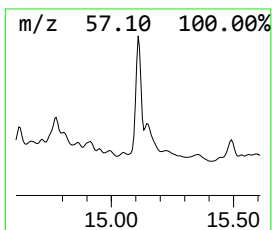
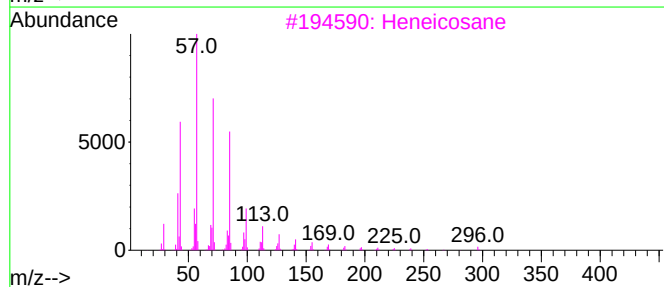
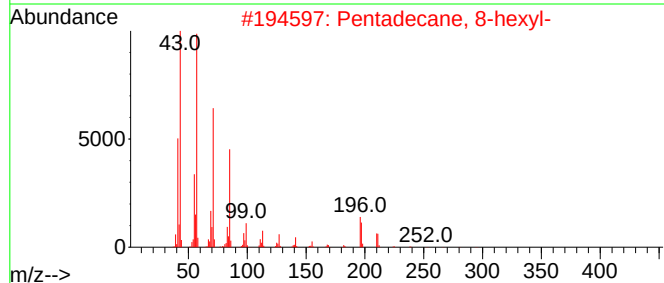
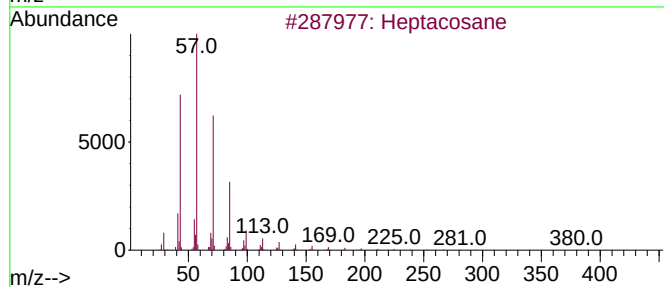
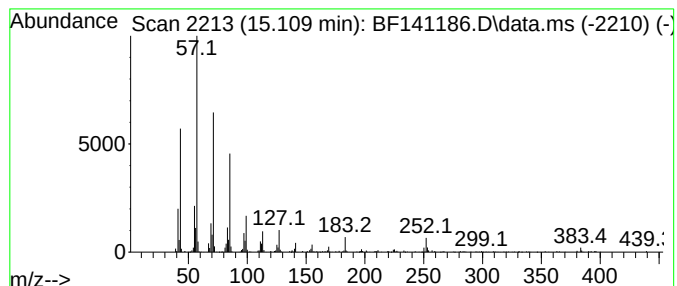
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.109	7.91 ng	301587	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	95
2			Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90
3			Heneicosane	296	C21H44	000629-94-7	90
4			Docosane	310	C22H46	000629-97-0	90
5			4-Methylheneicosane	310	C22H46	025117-29-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011625\
Data File : BF141186.D
Acq On : 16 Jan 2025 15:39
Operator : RC/JU
Sample : Q1094-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11938

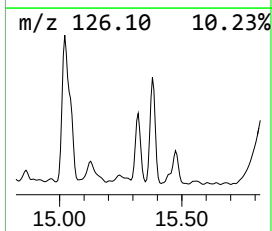
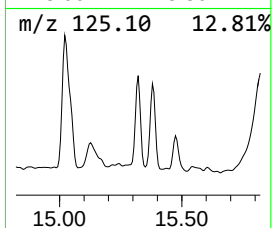
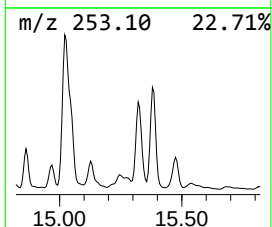
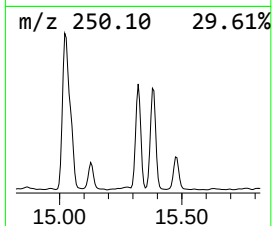
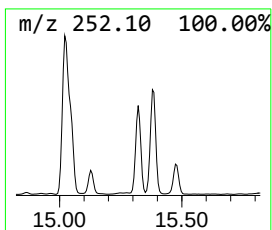
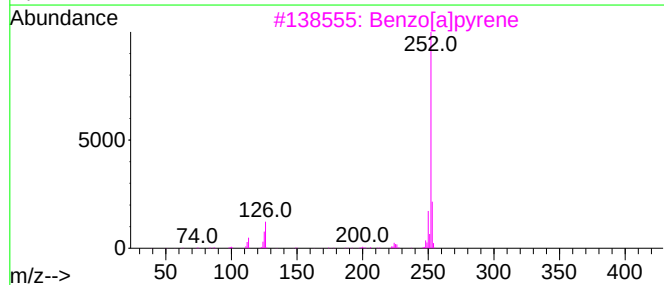
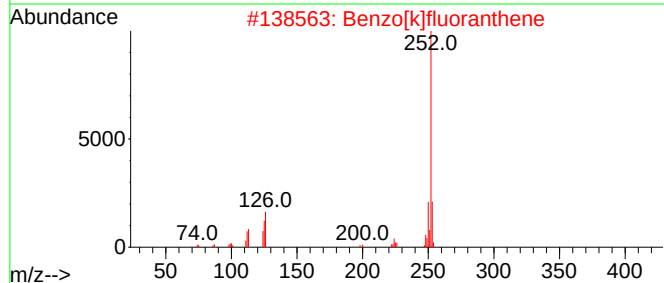
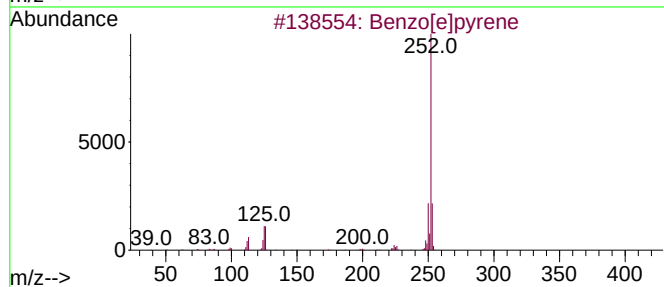
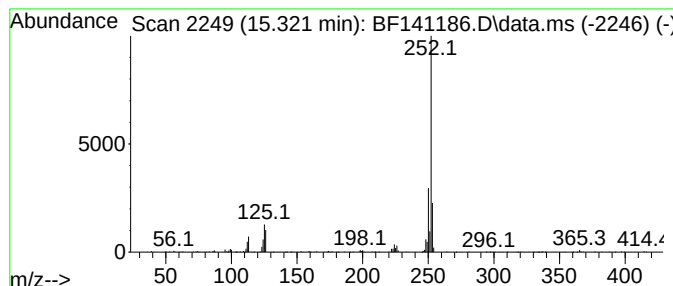
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.321	7.37 ng	280841	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	99
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
3			Benzo[a]pyrene	252	C20H12	000050-32-8	96
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	94
5			Perylene	252	C20H12	000198-55-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011625\
Data File : BF141186.D
Acq On : 16 Jan 2025 15:39
Operator : RC/JU
Sample : Q1094-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

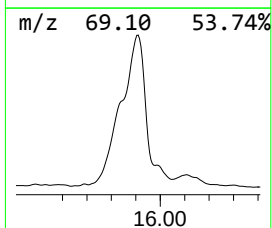
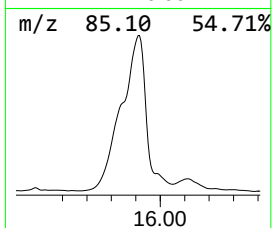
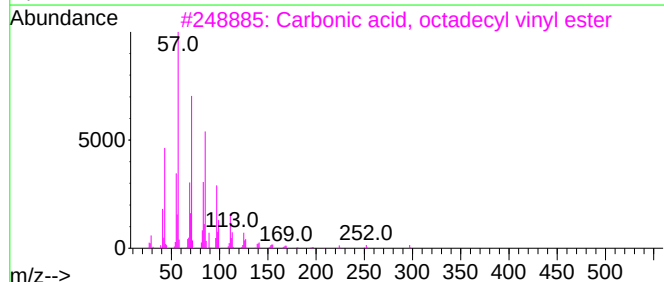
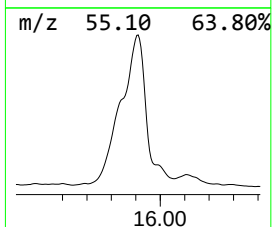
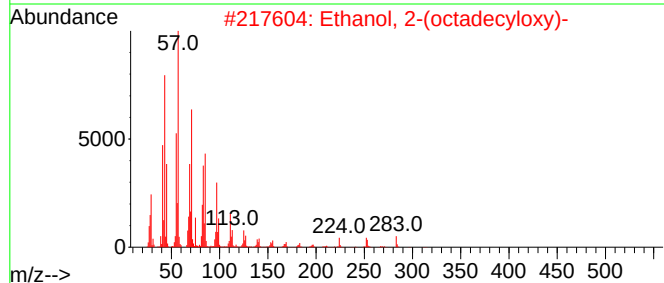
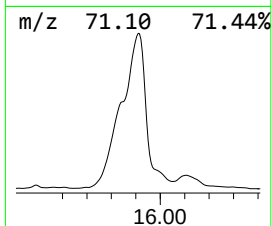
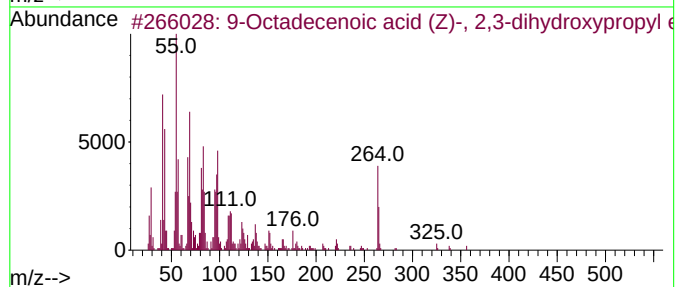
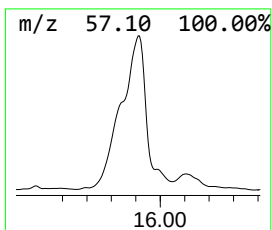
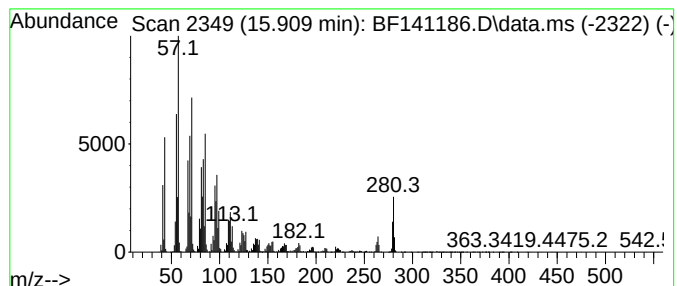
Instrument :
BNA_F
ClientSampleId :
72-11938

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 9-Octadecenoic acid (Z)-, 2... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.909	672.65 ng	25647800	Perylene-d12	15.445	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, 2,3-di...	356	C21H40O4	000111-03-5	64
2	Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	60
3	Carbonic acid, octadecyl vinyl e...	340	C21H40O3	1000382-54-4	60
4	Isobutyl hexadecyl ether	298	C20H42O	1000406-32-8	53
5	Isobutyl tetracosyl ether	410	C28H58O	1000406-33-2	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011625\
Data File : BF141186.D
Acq On : 16 Jan 2025 15:39
Operator : RC/JU
Sample : Q1094-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11938

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.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
Butane, 2-metho...	2.128	46.1	ng	2200580	1	6.816	955202	20.0
2-Pentanone, 4-...	5.045	8.9	ng	424938	1	6.816	955202	20.0
Benzophenone	10.569	7.9	ng	550267	3	9.851	1399350	20.0
4H-Cyclopenta[d...	11.957	4.5	ng	257878	4	11.339	1141860	20.0
Octadecanoic acid	12.668	21.8	ng	2143170	5	13.980	1966350	20.0
5-Eicosene, (E)-	13.839	4.2	ng	407830	5	13.980	1966350	20.0
Heptacosane	15.109	7.9	ng	301587	6	15.445	762586	20.0
Benzo[e]pyrene	15.321	7.4	ng	280841	6	15.445	762586	20.0
9-Octadecenoic ...	15.909	672.6	ng	25647800	6	15.445	762586	20.0