

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
 Data File : BF139191.D
 Acq On : 27 Aug 2024 17:21
 Operator : RC/JU
 Sample : P3732-03
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 UI-3

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-BF082724.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139191.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	8	15	22	rVB	1091010	1707800	87.26%	9.827%
2	3.387	211	220	245	rBV	46057	120901	6.18%	0.696%
3	5.104	504	512	521	rVB	79379	120530	6.16%	0.694%
4	5.504	574	580	585	rBV	1364513	1803721	92.16%	10.379%
5	6.510	745	751	756	rBV	1368513	1845386	94.29%	10.619%
6	6.710	781	785	796	rBV	60662	77153	3.94%	0.444%
7	6.893	811	816	821	rBV	397919	495965	25.34%	2.854%
8	7.451	905	911	916	rBV	912503	1164186	59.48%	6.699%
9	7.704	950	954	958	rBV	26991	30840	1.58%	0.177%
10	8.169	1028	1033	1038	rBV	494727	621065	31.73%	3.574%
11	8.481	1081	1086	1096	rBV	108836	136530	6.98%	0.786%
12	9.245	1211	1216	1221	rBV	1618401	1957169	100.00%	11.262%
13	9.922	1326	1331	1336	rBV	548802	675894	34.53%	3.889%
14	10.022	1341	1348	1357	rBV	418350	641347	32.77%	3.690%
15	10.710	1459	1465	1477	rBV	925602	1161472	59.34%	6.683%
16	11.410	1579	1584	1592	rBV2	491903	735437	37.58%	4.232%
17	11.480	1592	1596	1600	rVB	18083	22216	1.14%	0.128%
18	11.933	1664	1673	1678	rBV3	74857	118673	6.06%	0.683%
19	12.022	1684	1688	1696	rVB2	25021	47346	2.42%	0.272%
20	12.222	1715	1722	1727	rVB3	11489	24288	1.24%	0.140%
21	12.510	1765	1771	1774	rBV2	14907	22252	1.14%	0.128%
22	12.622	1782	1790	1794	rBV	172748	221326	11.31%	1.274%
23	12.845	1821	1828	1834	rBV	148580	216015	11.04%	1.243%
24	12.992	1843	1853	1858	rBV	1223854	1545237	78.95%	8.892%
25	13.174	1876	1884	1889	rBV	16540	31337	1.60%	0.180%
26	13.680	1960	1970	1975	rVV2	13346	23233	1.19%	0.134%
27	13.792	1984	1989	1992	rBV2	14533	24777	1.27%	0.143%
28	13.845	1992	1998	2002	rVV4	17188	38821	1.98%	0.223%
29	13.892	2002	2006	2017	rVB2	60787	105829	5.41%	0.609%
30	14.045	2024	2032	2043	rVB2	440288	731057	37.35%	4.207%
31	14.427	2088	2097	2100	rBV2	14973	26459	1.35%	0.152%
32	14.527	2108	2114	2116	rBV6	14586	23702	1.21%	0.136%
33	14.916	2175	2180	2188	rBV6	9180	21095	1.08%	0.121%
34	15.086	2203	2209	2219	rBV	76798	170331	8.70%	0.980%
35	15.192	2220	2227	2236	rVB3	12276	27673	1.41%	0.159%
36	15.392	2256	2261	2266	rVB	36061	54818	2.80%	0.315%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139191.D
Acq On : 27 Aug 2024 17:21
Operator : RC/JU
Sample : P3732-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UI-3

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-BF082724.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.451	2266	2271	2276	rVV	51182	76525	3.91%	0.440%
38	15.515	2276	2282	2297	rVB	272519	438977	22.43%	2.526%
39	16.986	2526	2532	2540	rVB2	17654	37517	1.92%	0.216%
40	17.427	2601	2607	2619	rBV	14542	33729	1.72%	0.194%

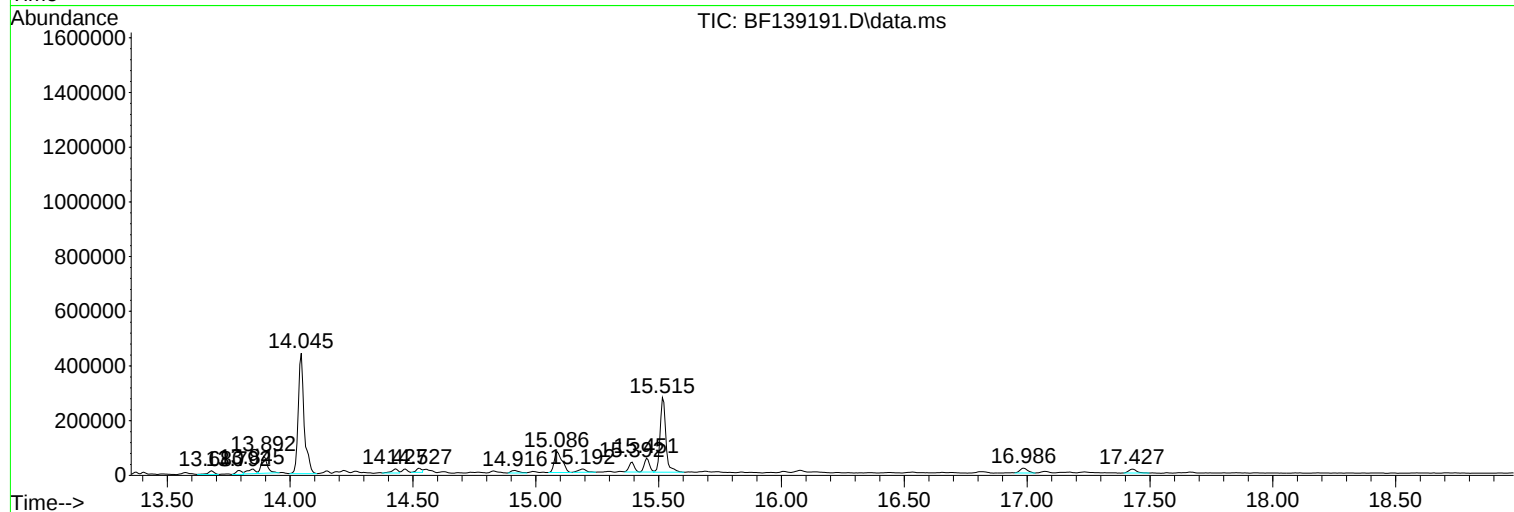
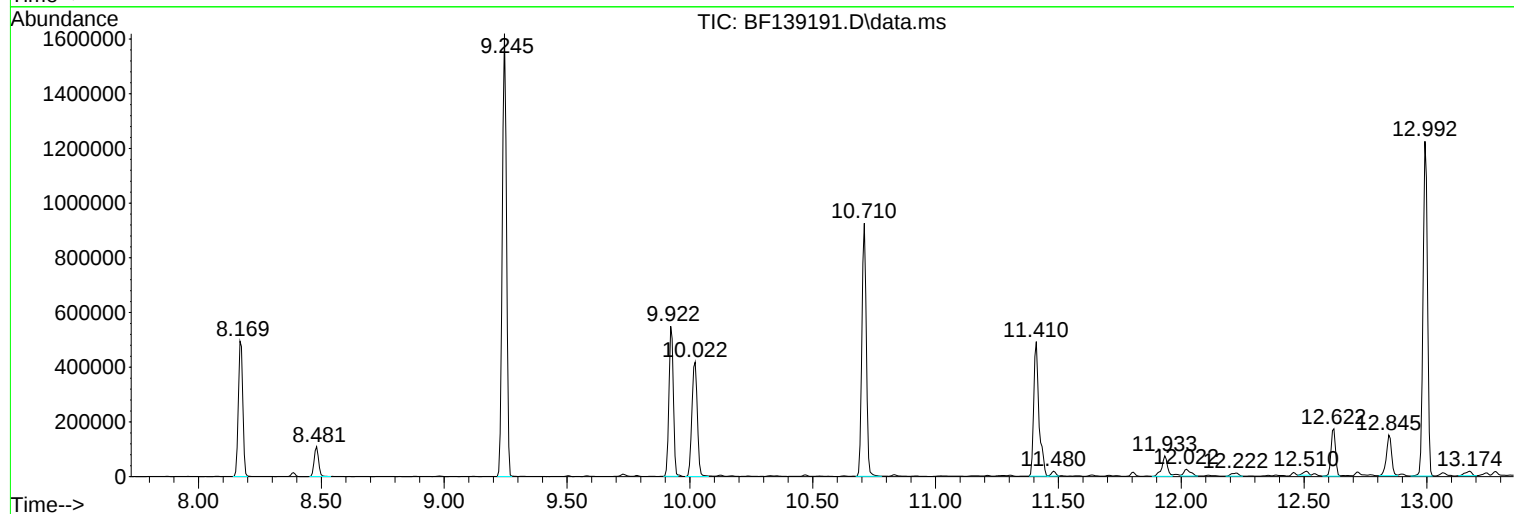
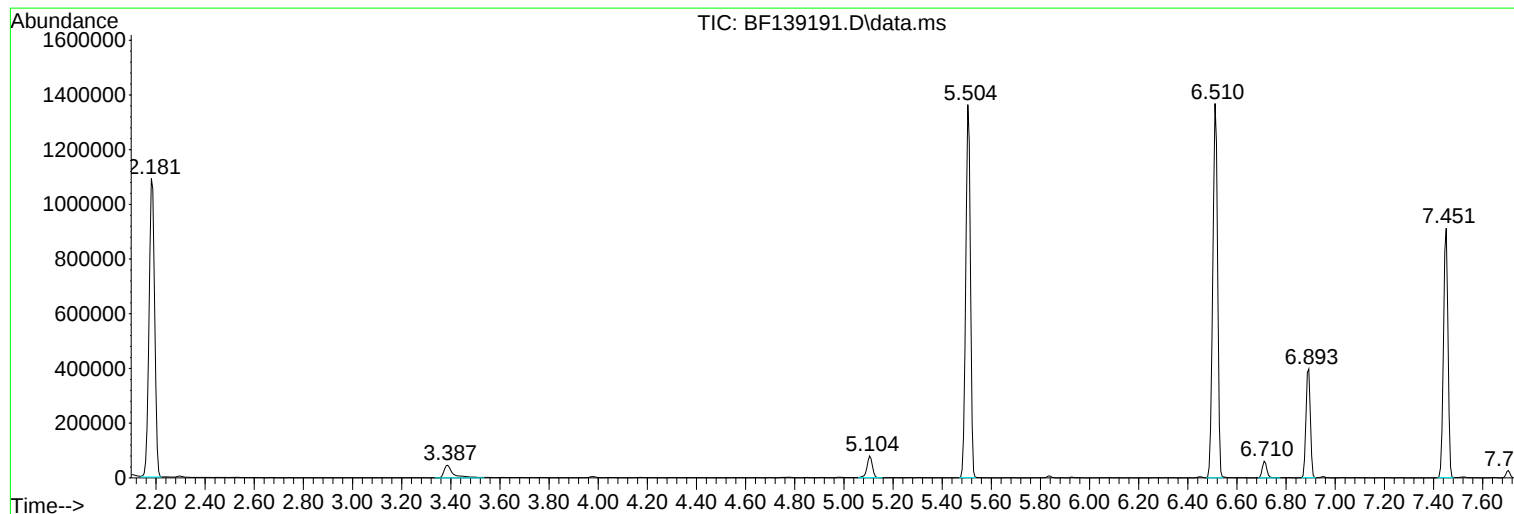
Sum of corrected areas: 17378629

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139191.D
Acq On : 27 Aug 2024 17:21
Operator : RC/JU
Sample : P3732-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UI-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.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\BF082724\
Data File : BF139191.D
Acq On : 27 Aug 2024 17:21
Operator : RC/JU
Sample : P3732-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UI-3

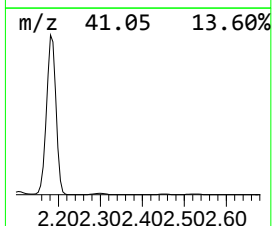
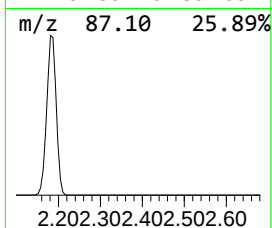
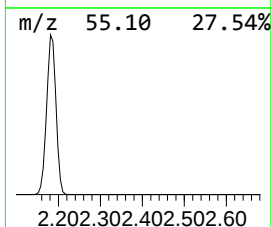
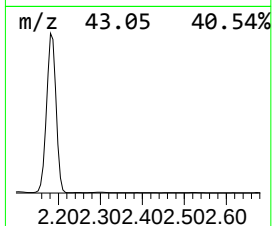
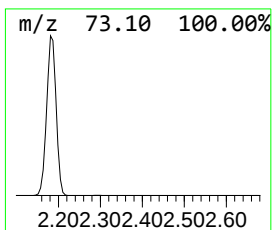
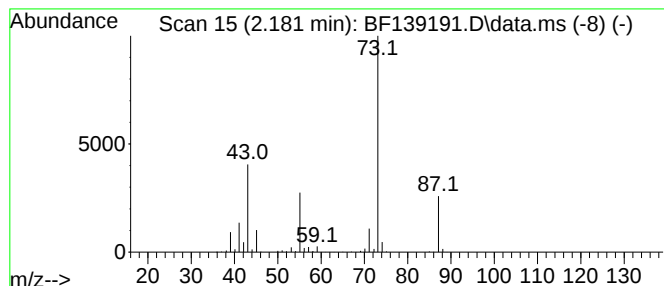
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	68.87 ng	1707800	1,4-Dichlorobenzene-d4	6.893

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	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139191.D
Acq On : 27 Aug 2024 17:21
Operator : RC/JU
Sample : P3732-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UI-3

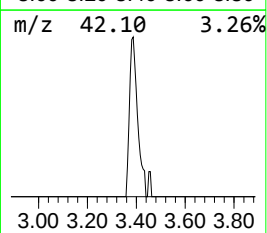
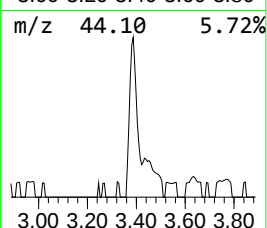
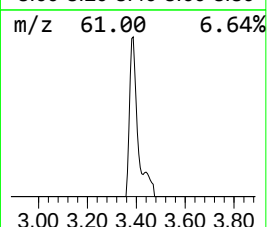
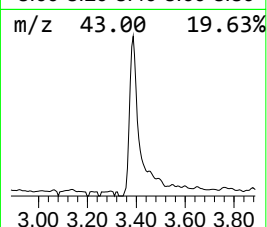
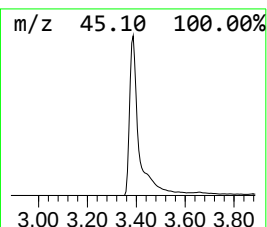
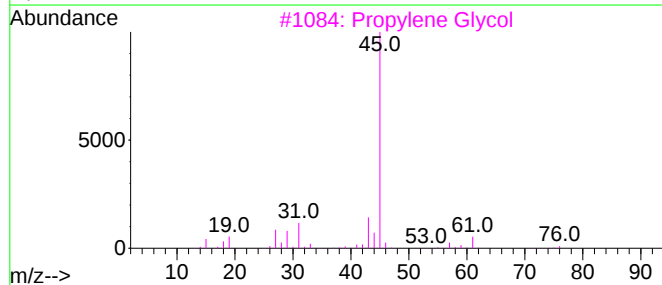
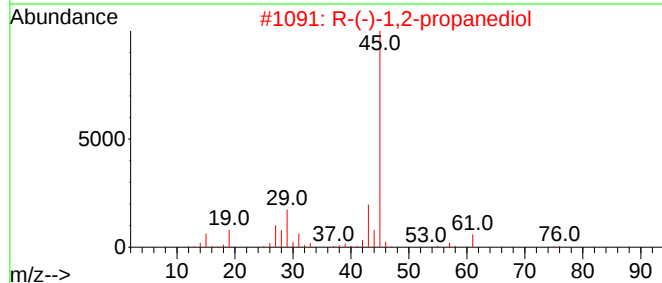
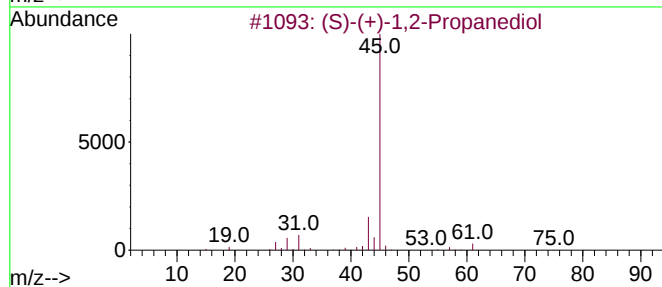
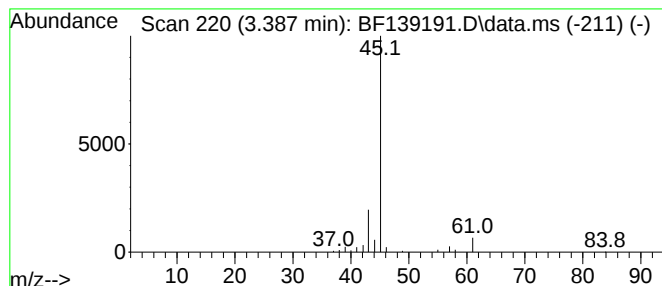
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.387	4.88 ng	120901	1,4-Dichlorobenzene-d4	6.893

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
3		Propylene Glycol	76	C3H8O2	000057-55-6	9
4		Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5		Formamide	45	CH3NO	000075-12-7	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139191.D
Acq On : 27 Aug 2024 17:21
Operator : RC/JU
Sample : P3732-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UI-3

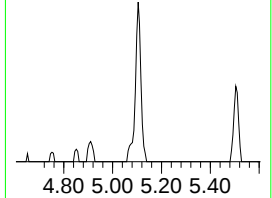
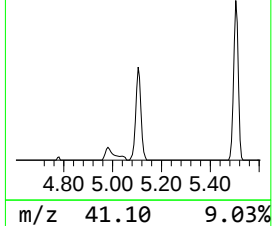
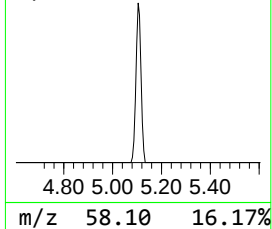
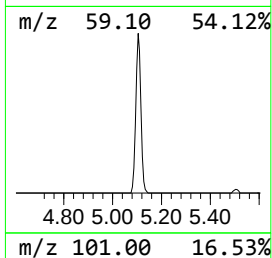
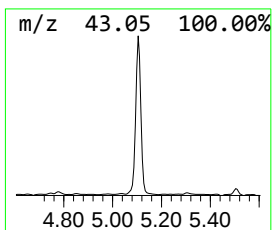
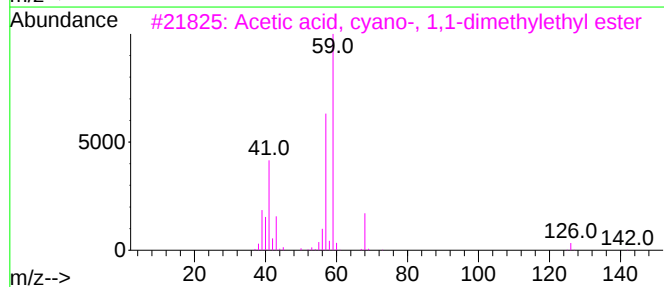
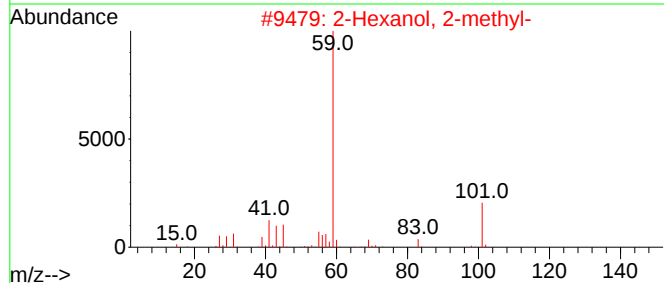
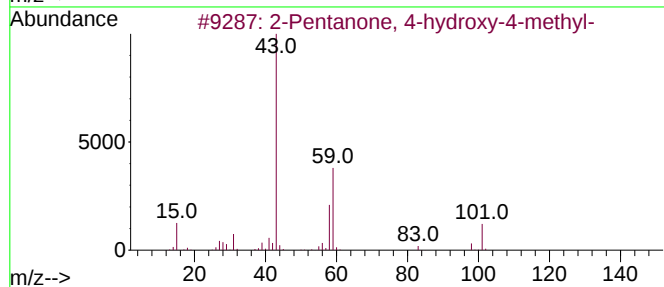
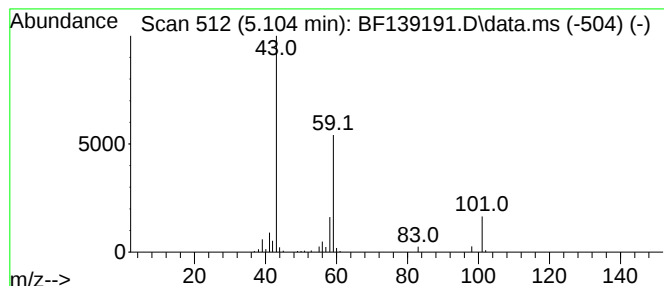
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	4.86 ng	120530	1,4-Dichlorobenzene-d4	6.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139191.D
Acq On : 27 Aug 2024 17:21
Operator : RC/JU
Sample : P3732-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UI-3

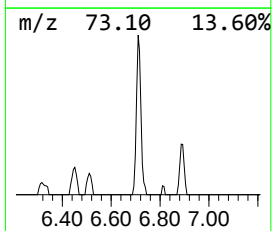
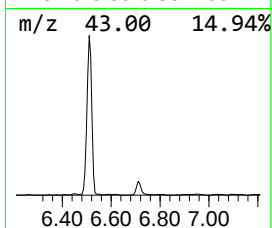
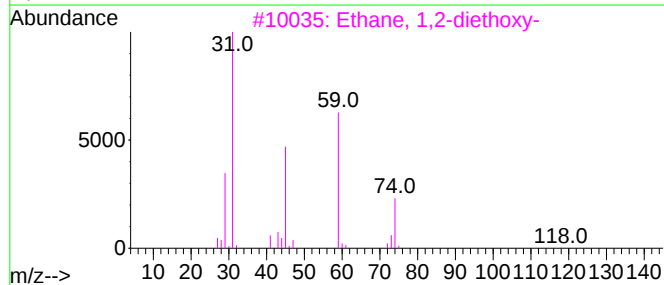
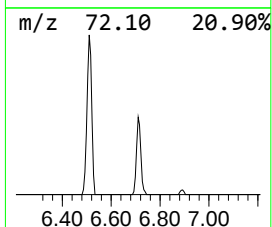
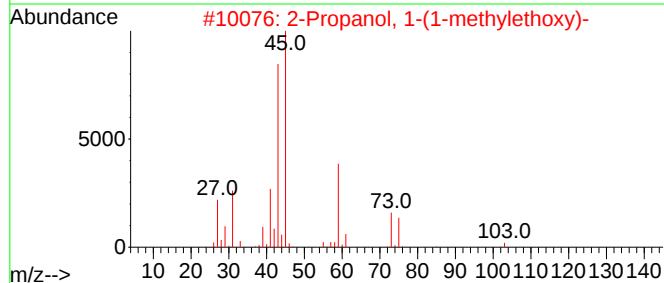
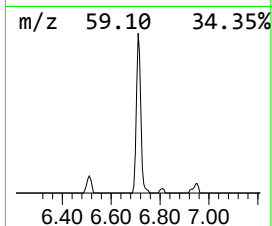
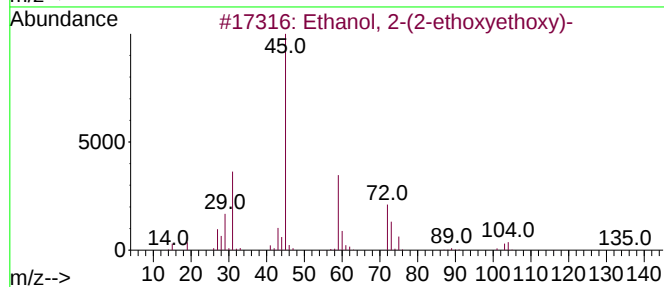
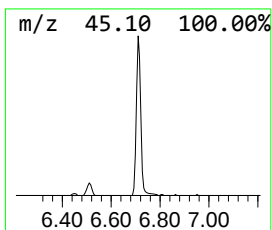
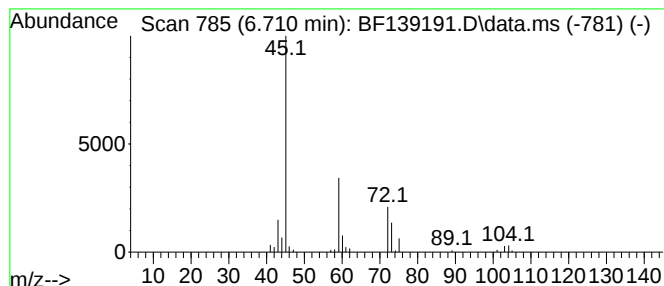
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.710	3.11 ng	77153	1,4-Dichlorobenzene-d4	6.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	39
3			Ethane, 1,2-diethoxy-	118	C6H14O2	000629-14-1	36
4			Carbonic acid, dimethyl ester	90	C3H6O3	000616-38-6	36
5			Ethyl ether	74	C4H10O	000060-29-7	33



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139191.D
Acq On : 27 Aug 2024 17:21
Operator : RC/JU
Sample : P3732-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UI-3

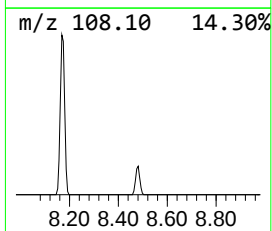
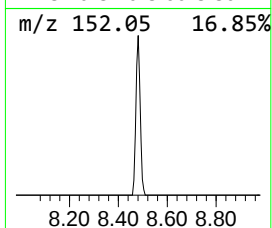
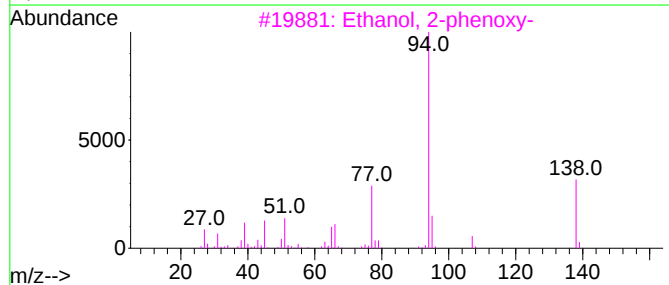
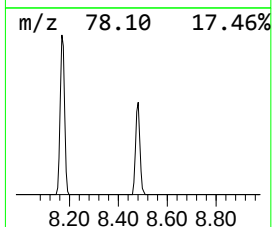
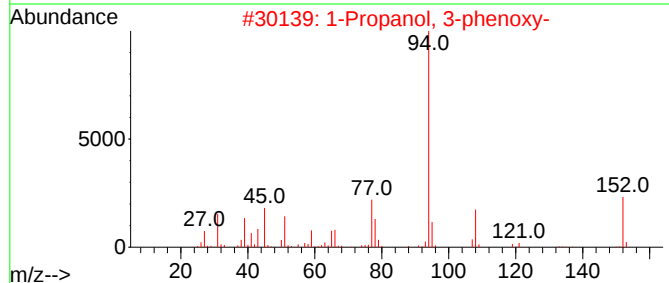
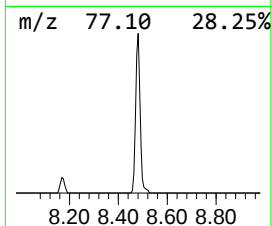
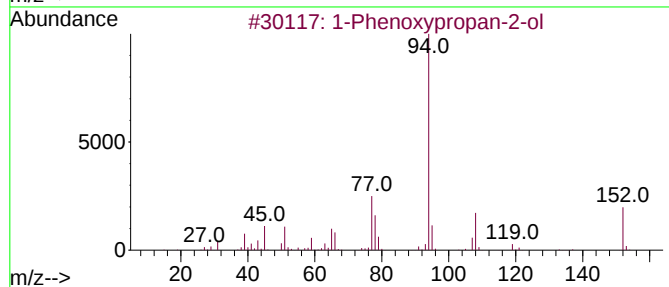
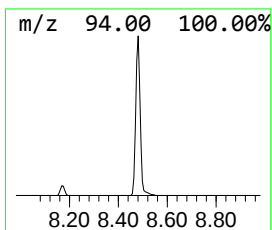
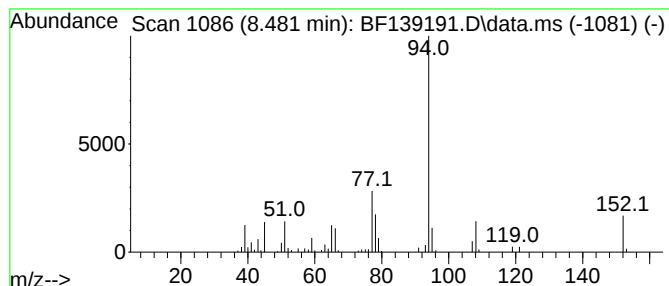
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.481	4.40 ng	136530	Naphthalene-d8	8.169

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	97
2		1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3		Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4		Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59
5		1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139191.D
Acq On : 27 Aug 2024 17:21
Operator : RC/JU
Sample : P3732-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UI-3

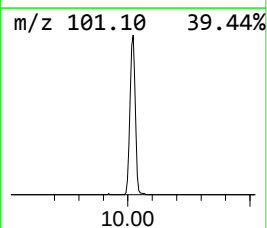
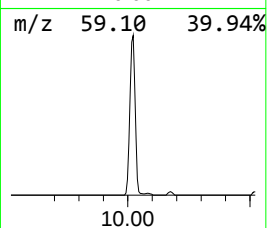
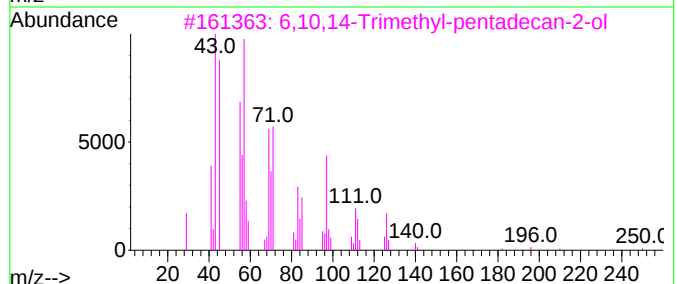
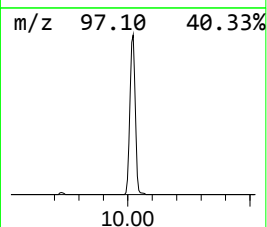
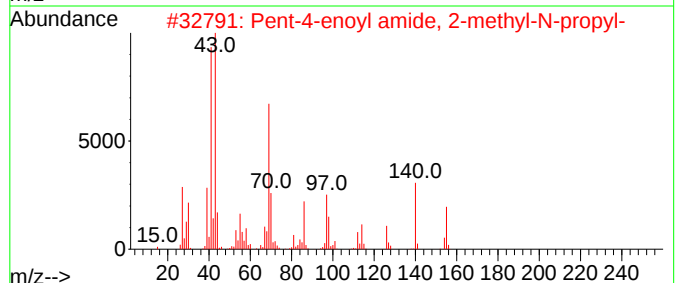
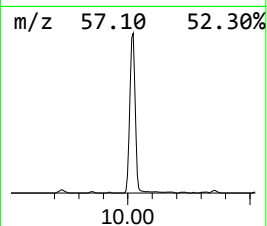
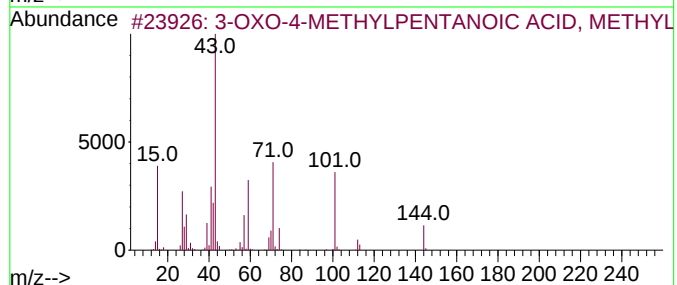
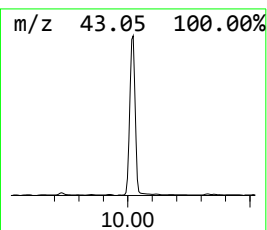
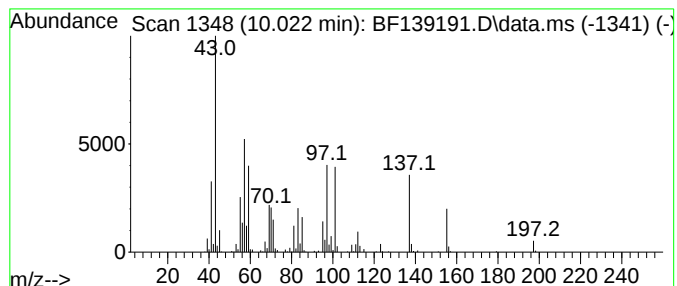
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown10.022 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.022	18.98 ng	641347	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-OXO-4-METHYLPENTANOIC ACID, ME...	144	C7H12O3	042558-54-3	16
2			Pent-4-enoyl amide, 2-methyl-N-p...	155	C9H17NO	1000420-35-2	14
3			6,10,14-Trimethyl-pentadecan-2-ol	270	C18H38O	069729-17-5	12
4			2-Chloropropionic acid, decyl e...	248	C13H25ClO2	086711-78-6	10
5			1-Tridecene	182	C13H26	002437-56-1	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139191.D
Acq On : 27 Aug 2024 17:21
Operator : RC/JU
Sample : P3732-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UI-3

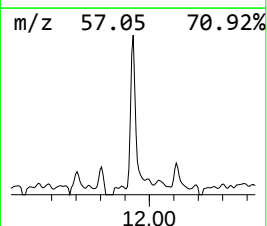
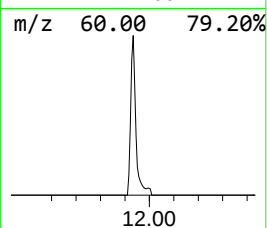
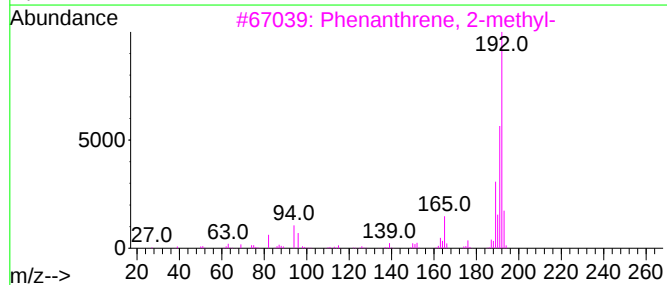
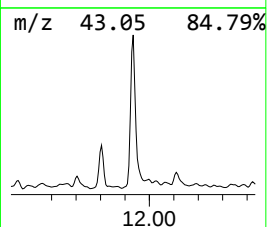
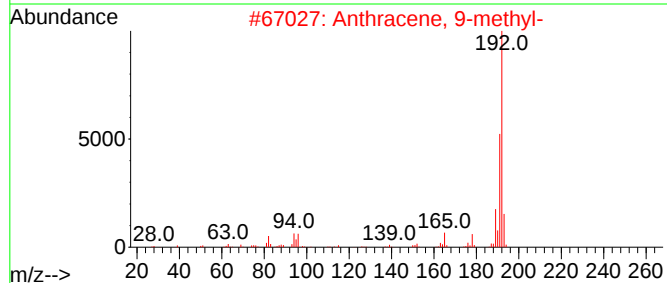
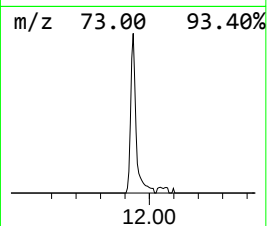
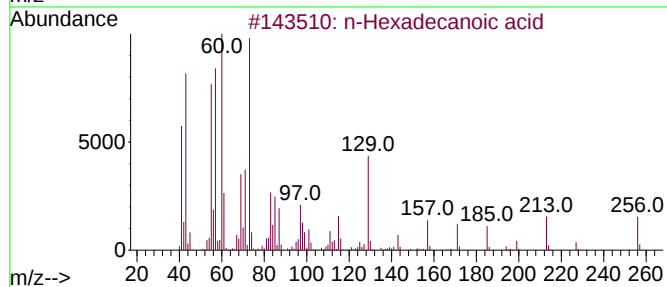
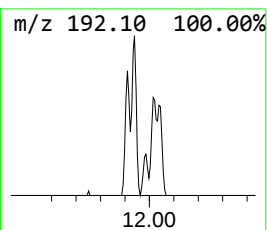
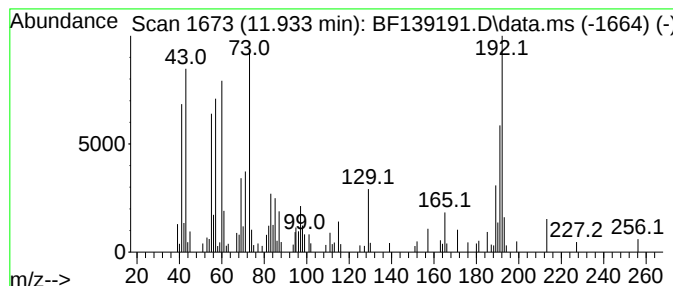
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	3.23 ng	118673	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Anthracene, 9-methyl-	192	C15H12	000779-02-2	92
3			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	92
4			Anthracene, 2-methyl-	192	C15H12	000613-12-7	87
5			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139191.D
Acq On : 27 Aug 2024 17:21
Operator : RC/JU
Sample : P3732-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UI-3

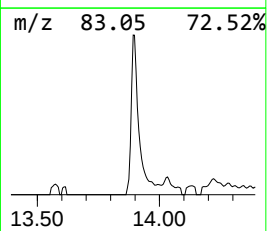
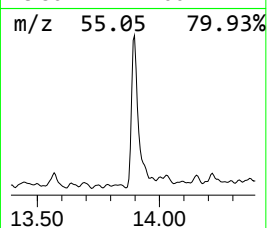
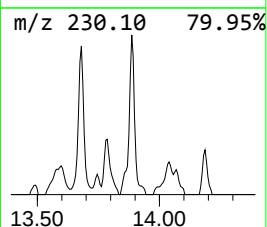
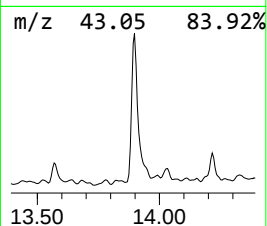
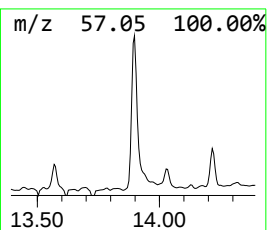
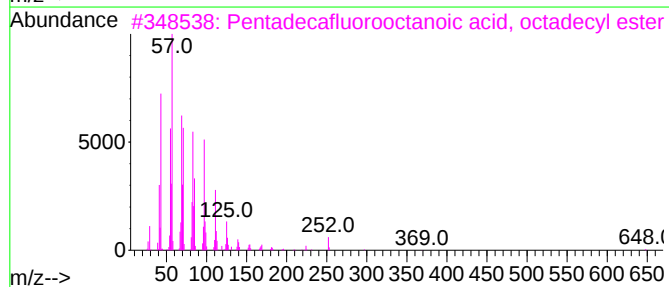
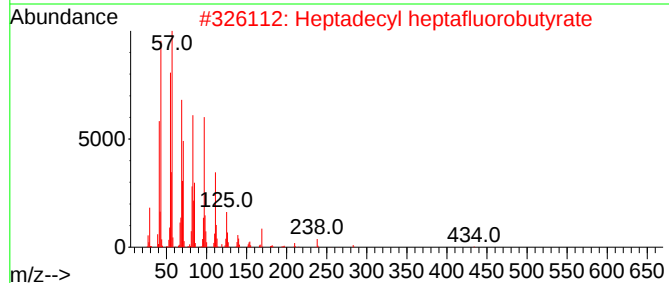
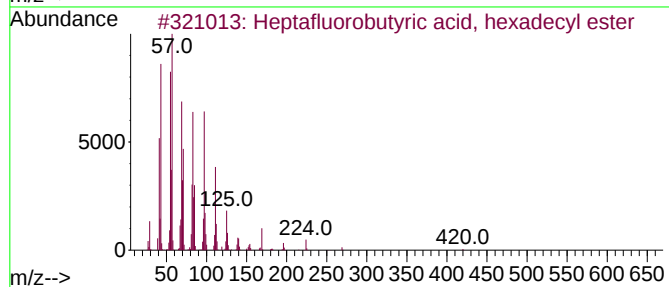
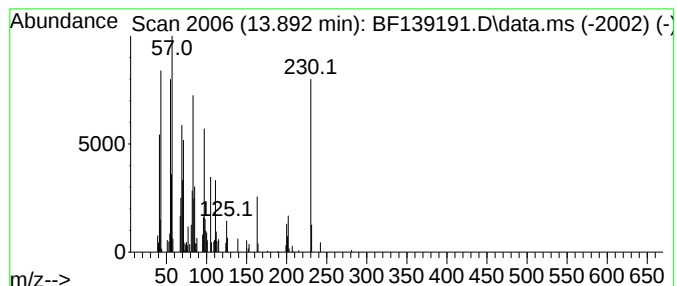
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptafluorobutyric acid, he... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	2.90 ng	105829	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	90
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	90
4			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	86
5			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139191.D
Acq On : 27 Aug 2024 17:21
Operator : RC/JU
Sample : P3732-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UI-3

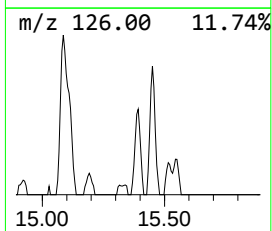
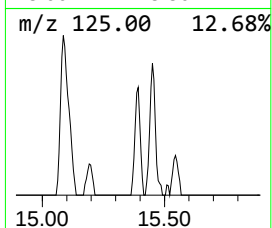
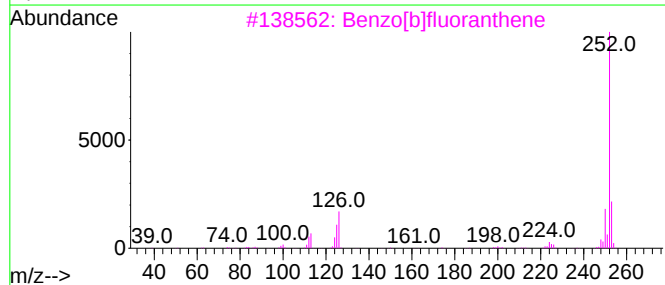
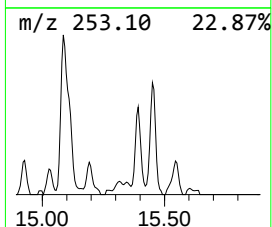
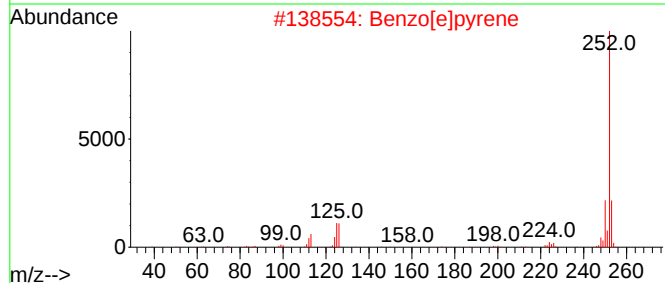
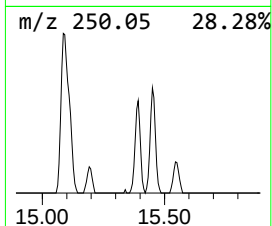
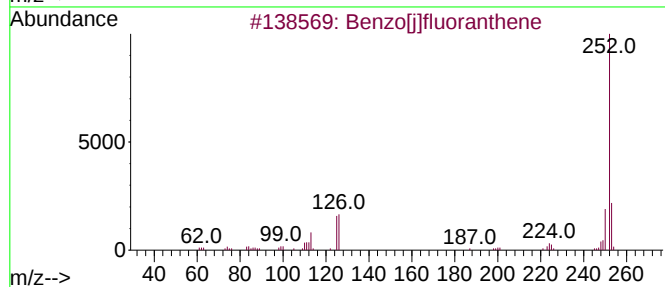
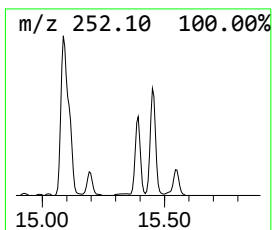
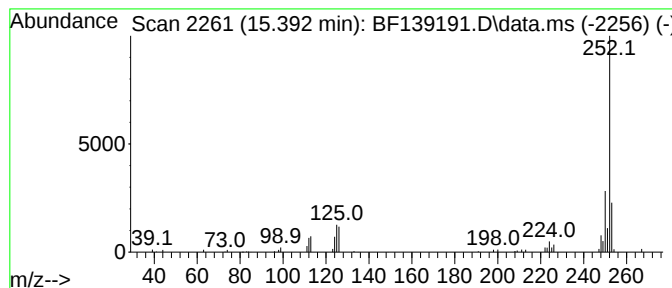
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzo[j]fluoranthene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.392	2.50 ng	54818	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[j]fluoranthene	252	C20H12	000205-82-3	95
2			Benzo[e]pyrene	252	C20H12	000192-97-2	94
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
4			Benzo[a]pyrene	252	C20H12	000050-32-8	90
5			Perylene	252	C20H12	000198-55-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139191.D
Acq On : 27 Aug 2024 17:21
Operator : RC/JU
Sample : P3732-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UI-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.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...	2.181	68.9	ng	1707800	1	6.893	495965	20.0
(S)-(+)-1,2-Pro...	3.387	4.9	ng	120901	1	6.893	495965	20.0
2-Pentanone, 4-...	5.104	4.9	ng	120530	1	6.893	495965	20.0
Ethanol, 2-(2-e...	6.710	3.1	ng	77153	1	6.893	495965	20.0
1-Phenoxypropan...	8.481	4.4	ng	136530	2	8.169	621065	20.0
unknown10.022	10.022	19.0	ng	641347	3	9.922	675894	20.0
n-Hexadecanoic ...	11.933	3.2	ng	118673	4	11.410	735437	20.0
Heptafluorobuty...	13.892	2.9	ng	105829	5	14.045	731057	20.0
Benzo[j]fluoran...	15.392	2.5	ng	54818	6	15.515	438977	20.0