

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
 Data File : BF139194.D
 Acq On : 27 Aug 2024 18:56
 Operator : RC/JU
 Sample : P3735-07
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-13

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: BF139194.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.210	10	20	28	rVB	1147841	1830200	75.06%	9.724%
2	3.410	217	224	235	rBV	58971	125045	5.13%	0.664%
3	5.116	504	514	520	rVB	101919	168997	6.93%	0.898%
4	5.510	574	581	586	rBV	1756711	2350610	96.41%	12.489%
5	6.516	745	752	757	rBV	1661294	2386960	97.90%	12.683%
6	6.710	780	785	792	rBV	66671	84665	3.47%	0.450%
7	6.892	810	816	821	rBV	461074	574776	23.57%	3.054%
8	7.451	904	911	916	rBV	1142260	1483490	60.84%	7.882%
9	7.704	949	954	958	rBV	26300	31156	1.28%	0.166%
10	8.169	1028	1033	1039	rBV	553487	708678	29.07%	3.765%
11	8.481	1081	1086	1091	rBV	105906	132210	5.42%	0.702%
12	9.245	1210	1216	1221	rBV	1992143	2438224	100.00%	12.955%
13	9.922	1326	1331	1336	rBV	619066	757671	31.07%	4.026%
14	10.016	1341	1347	1354	rBV	140105	215998	8.86%	1.148%
15	10.710	1459	1465	1479	rBV	1123040	1407738	57.74%	7.480%
16	11.410	1579	1584	1591	rBV	506404	687244	28.19%	3.652%
17	11.933	1665	1673	1684	rBV3	71099	116138	4.76%	0.617%
18	12.021	1684	1688	1697	rVB3	14222	27378	1.12%	0.145%
19	12.616	1783	1789	1795	rBV	51319	68645	2.82%	0.365%
20	12.716	1802	1806	1813	rBV2	18551	28047	1.15%	0.149%
21	12.845	1819	1828	1834	rBV	47284	78216	3.21%	0.416%
22	12.992	1848	1853	1858	rBV	1425974	1777244	72.89%	9.443%
23	13.474	1930	1935	1942	rBV	74262	107477	4.41%	0.571%
24	13.898	2001	2007	2020	rBV2	62403	113157	4.64%	0.601%
25	14.045	2026	2032	2043	rVB	438979	631228	25.89%	3.354%
26	14.521	2109	2113	2118	rBV3	17837	29384	1.21%	0.156%
27	15.086	2205	2209	2219	rVB	24698	56959	2.34%	0.303%
28	15.515	2276	2282	2288	rBV	267972	403230	16.54%	2.142%

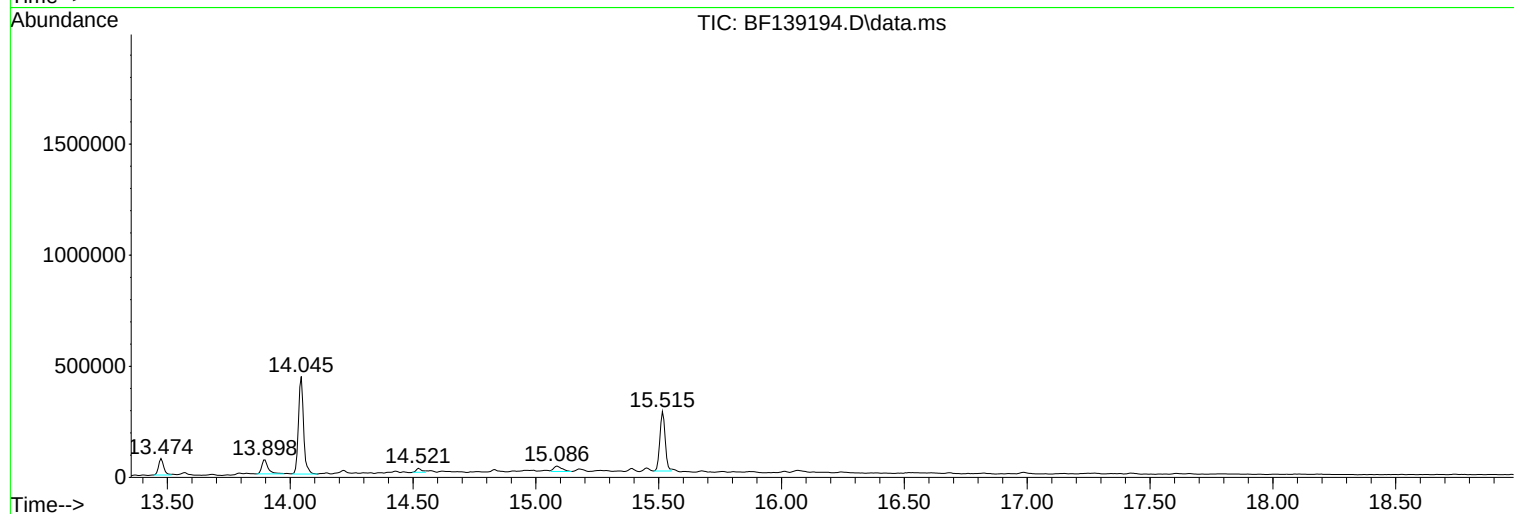
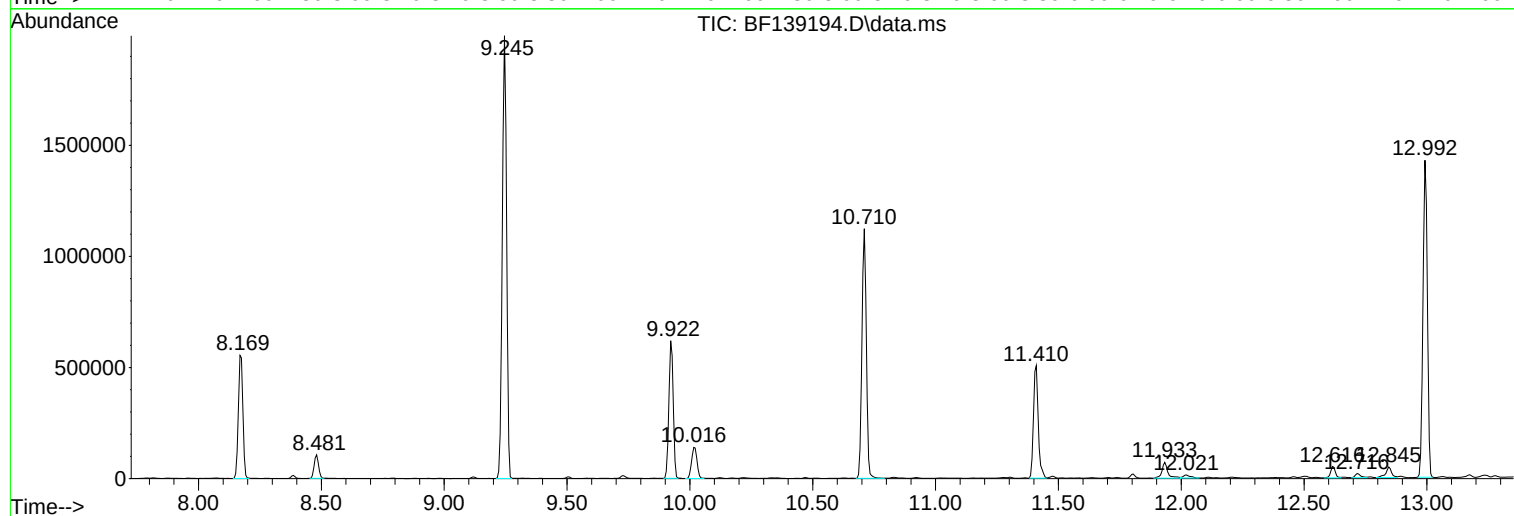
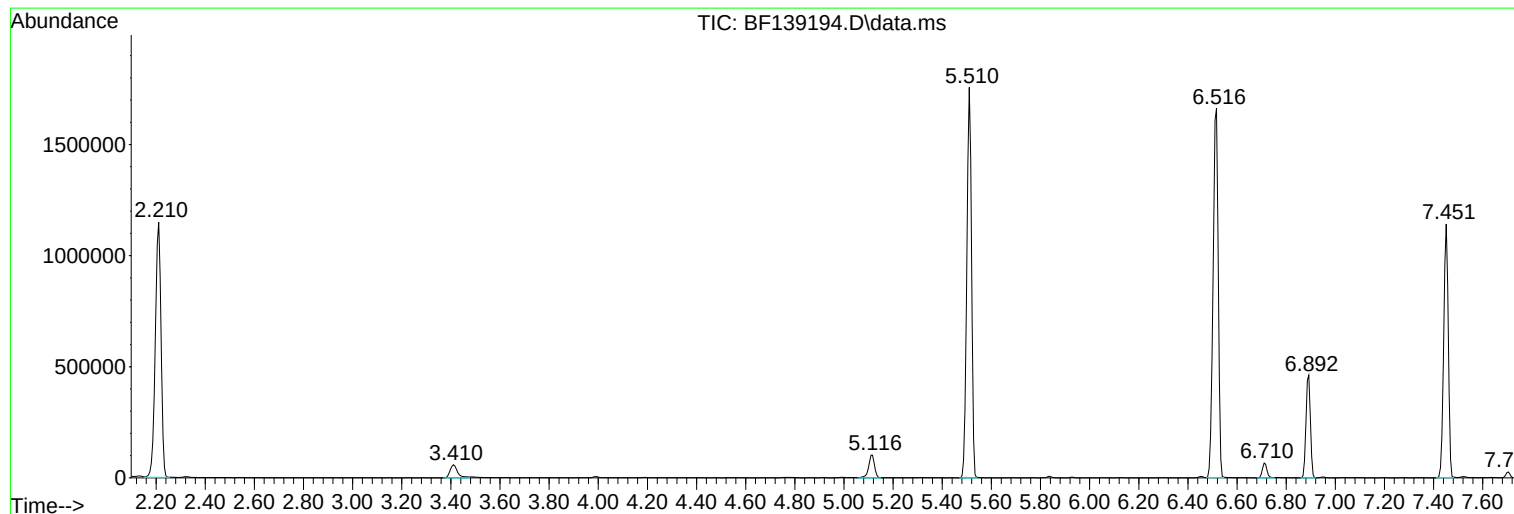
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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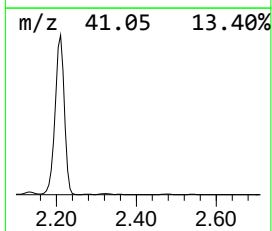
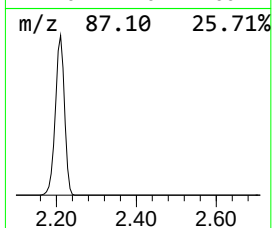
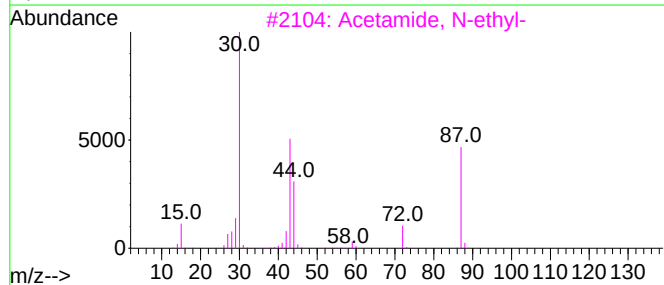
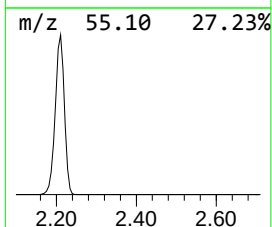
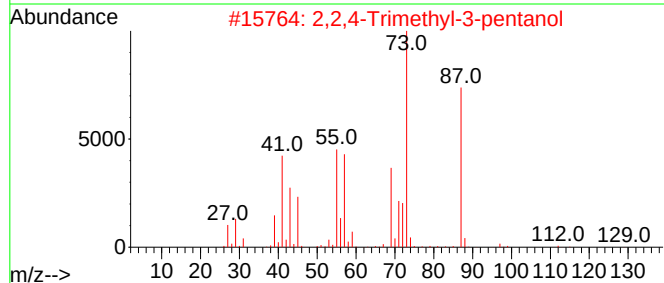
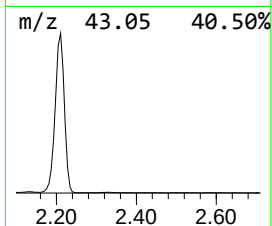
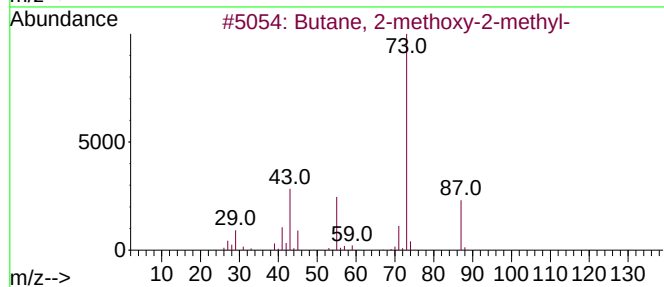
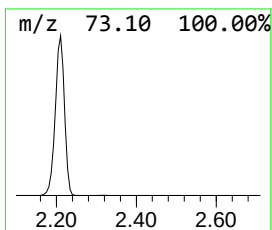
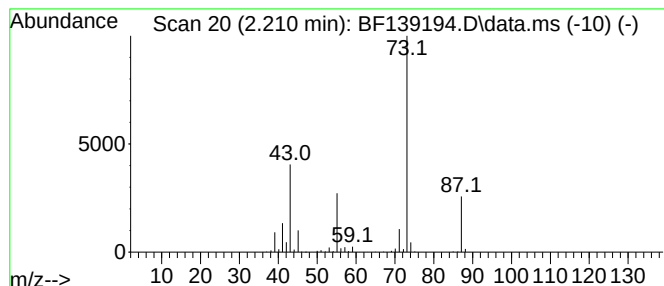
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.210	63.68 ng	1830200	1,4-Dichlorobenzene-d4	6.892

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			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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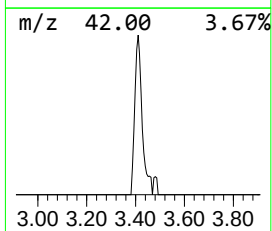
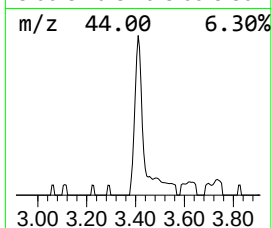
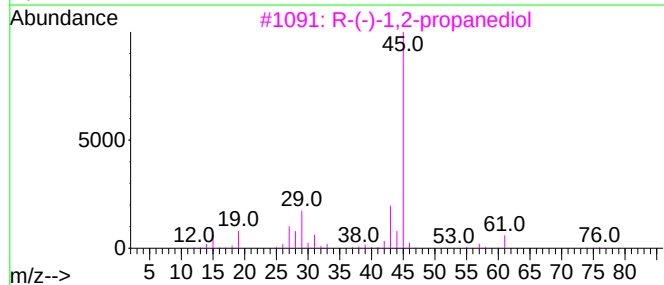
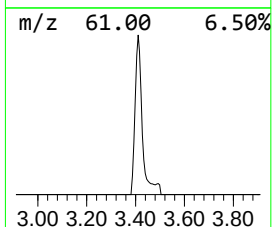
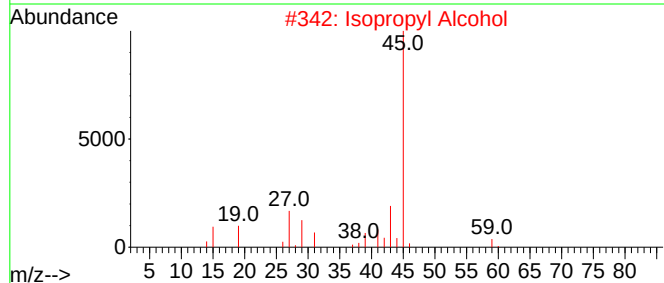
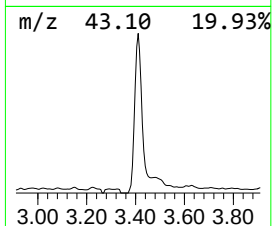
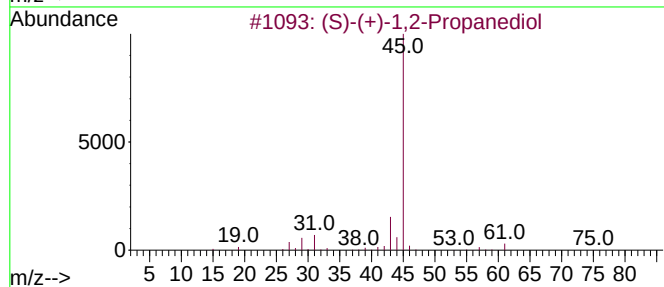
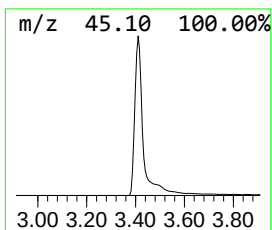
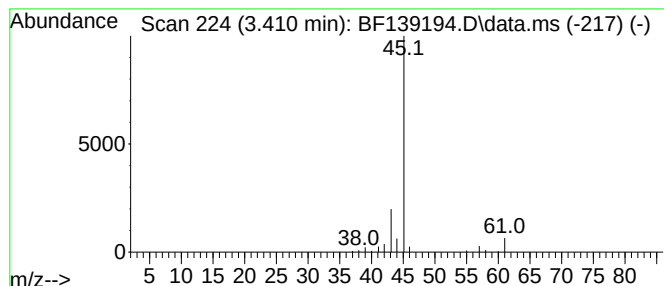
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.410	4.35 ng	125045	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol			76	C3H8O2	004254-15-3	64
2	Isopropyl Alcohol			60	C3H8O	000067-63-0	56
3	R-(-)-1,2-propanediol			76	C3H8O2	004254-14-2	43
4	Propylene Glycol			76	C3H8O2	000057-55-6	9
5	Formamide			45	CH3NO	000075-12-7	5



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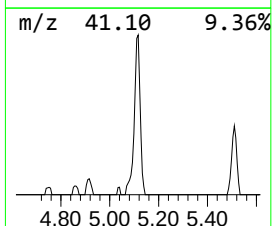
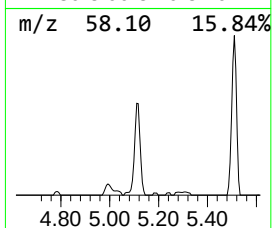
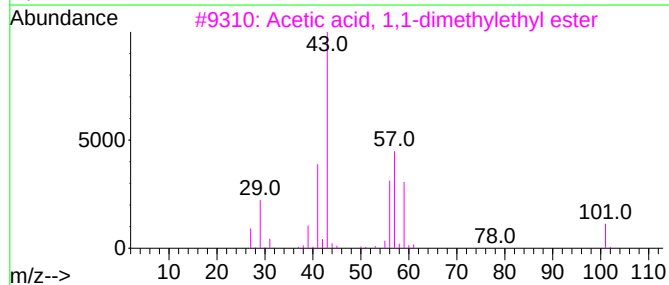
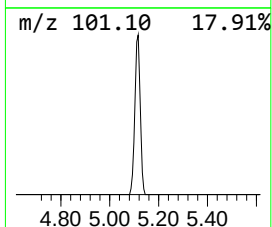
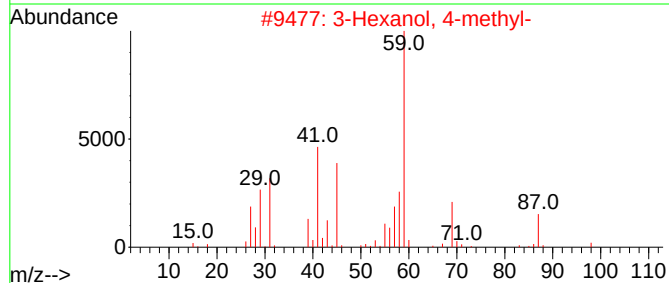
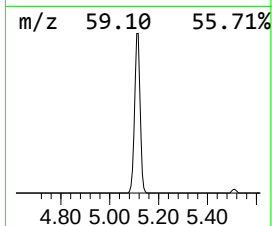
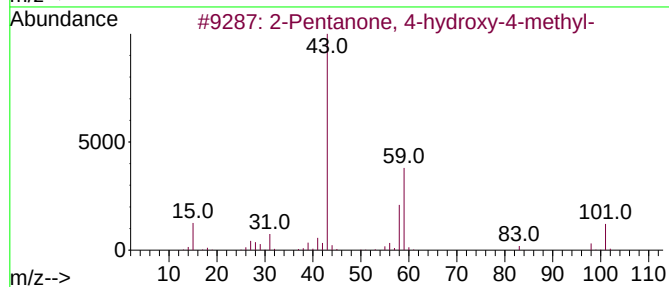
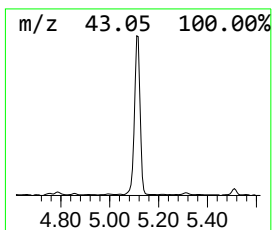
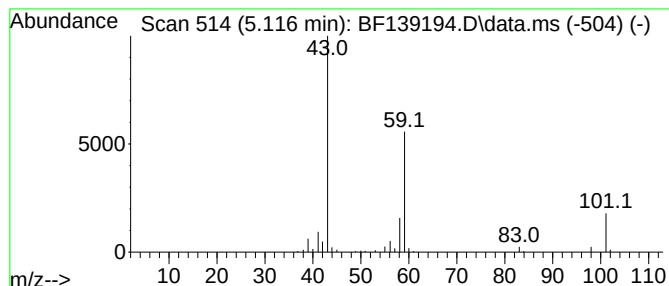
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	5.88 ng	168997	1,4-Dichlorobenzene-d4	6.892

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64	
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28	
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16	
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12	



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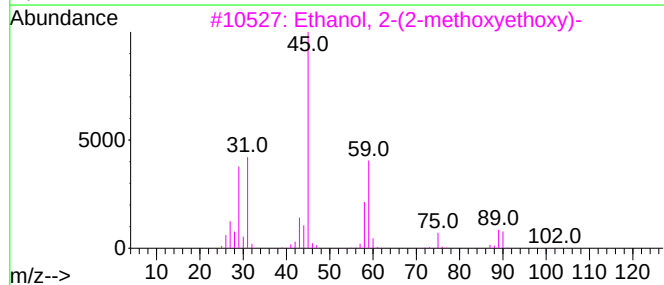
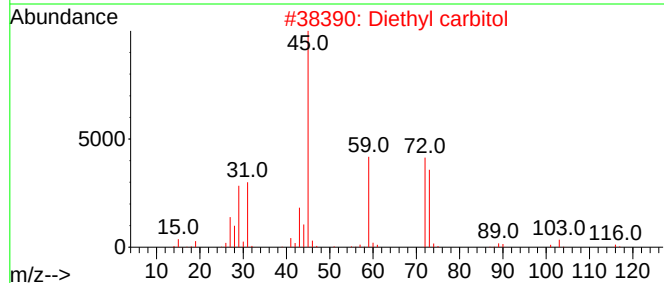
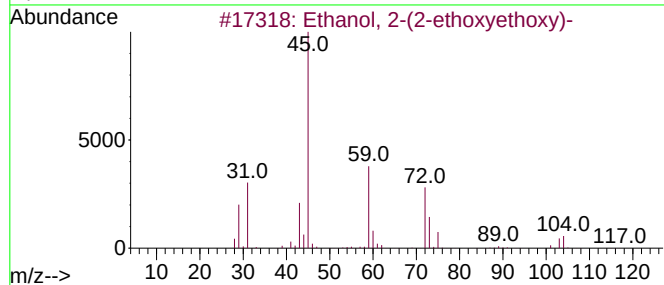
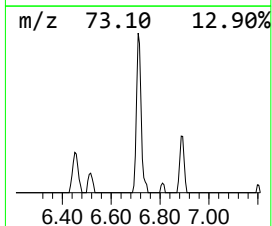
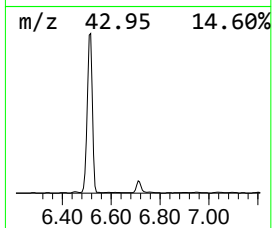
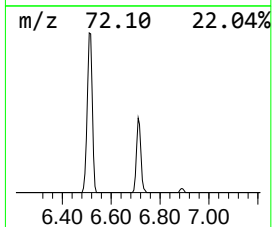
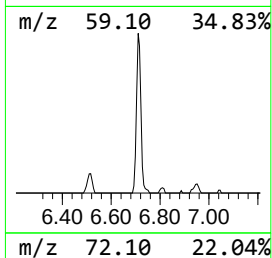
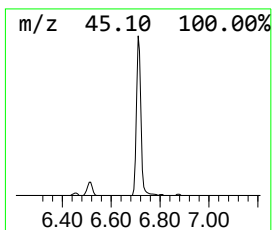
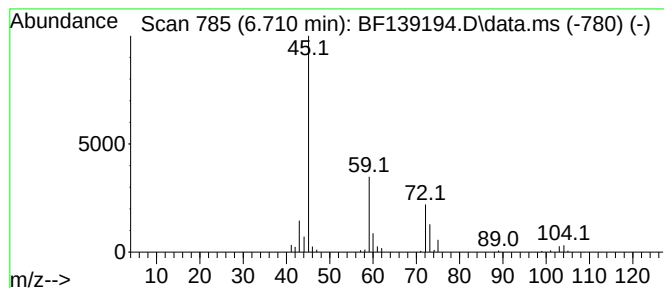
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.710	2.95 ng	84665	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2			Diethyl carbitol	162	C8H18O3	000112-36-7	78
3			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	45
4			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38
5			Ethane, 1,2-diethoxy-	118	C6H14O2	000629-14-1	36



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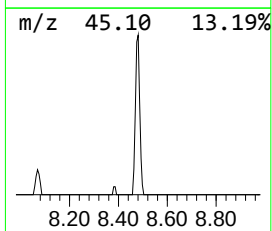
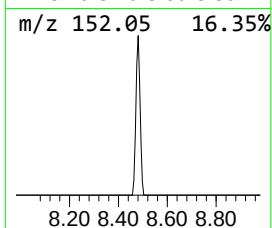
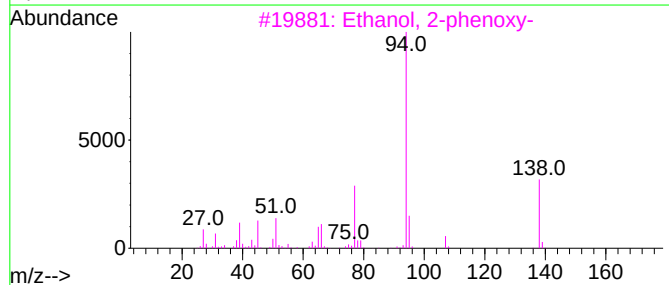
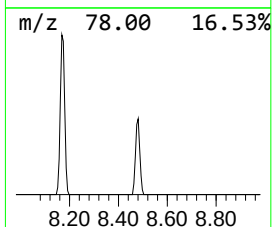
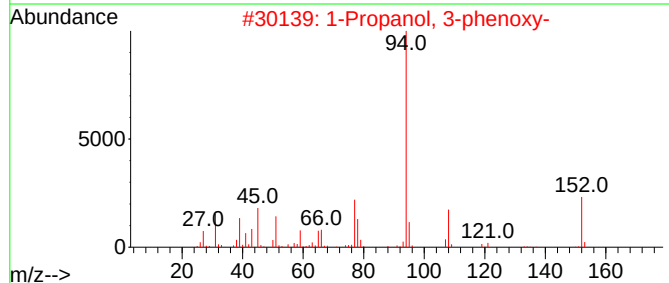
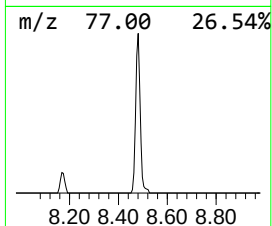
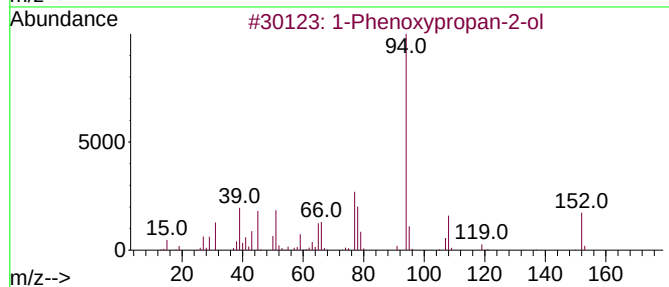
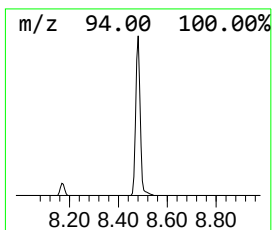
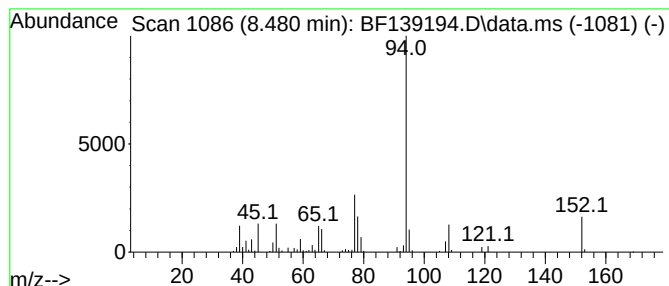
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.480	3.73 ng	132210	Naphthalene-d8	8.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59
5			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59



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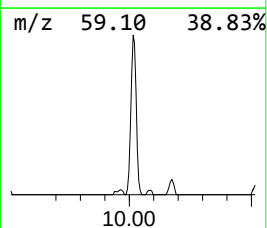
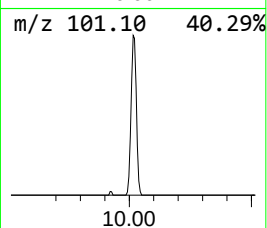
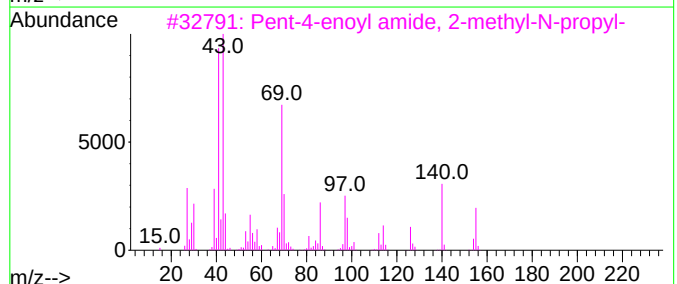
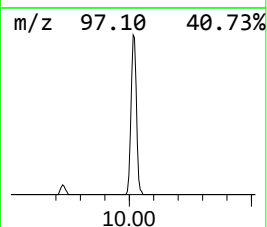
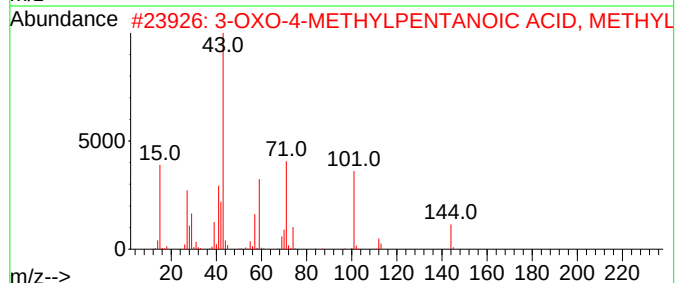
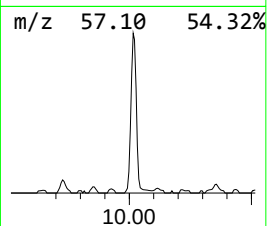
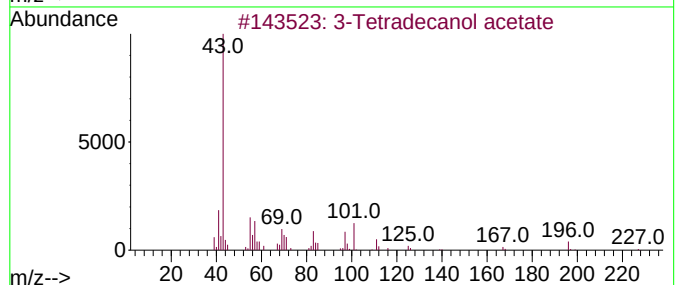
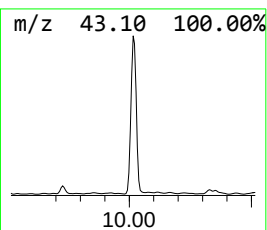
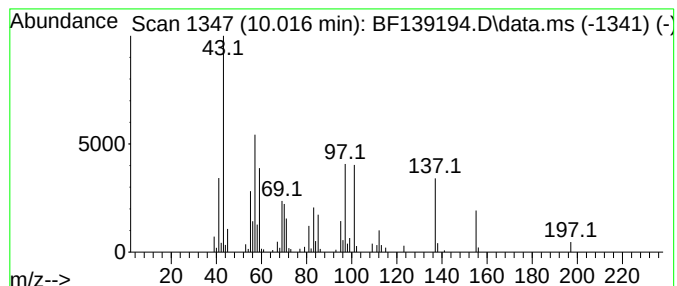
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown10.016 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.016	5.70 ng	215998	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Tetradecanol acetate	256	C16H32O2	051354-23-5	35
2			3-OXO-4-METHYLPENTANOIC ACID, ME...	144	C7H12O3	042558-54-3	16
3			Pent-4-enoyl amide, 2-methyl-N-p...	155	C9H17NO	1000420-35-2	14
4			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	10
5			2-Chloropropionic acid, decyl e...	248	C13H25ClO2	086711-78-6	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139194.D
Acq On : 27 Aug 2024 18:56
Operator : RC/JU
Sample : P3735-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-13

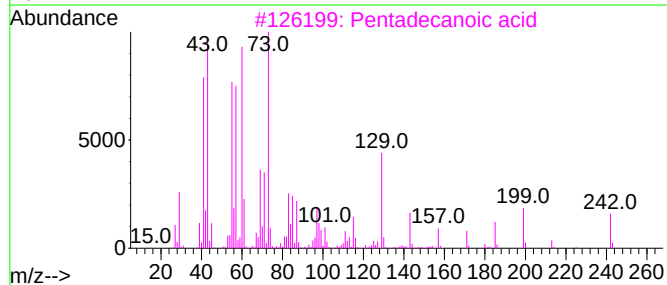
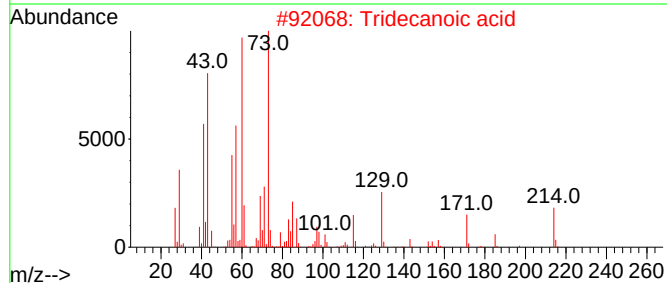
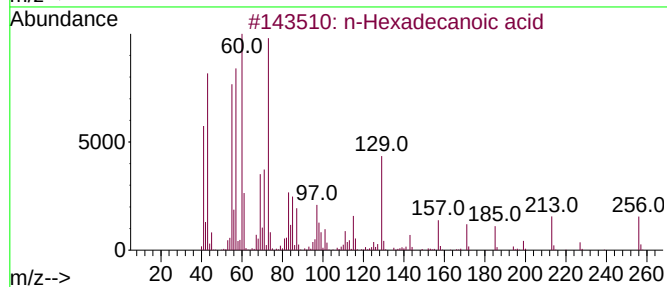
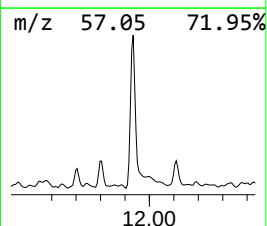
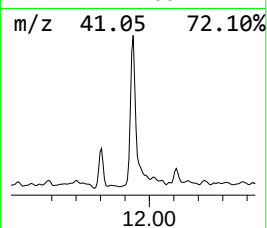
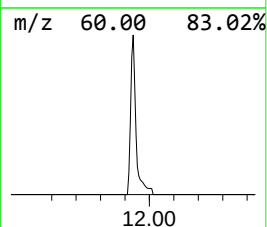
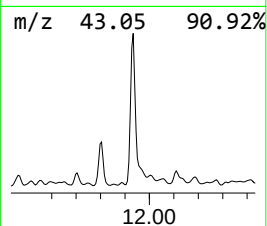
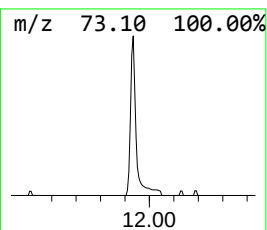
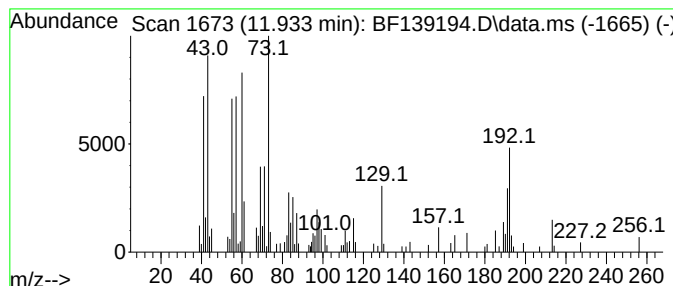
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	3.38 ng	116138	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	60
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	52
5			Acetamide, N-(4-hydroxycyclohexy...	157	C8H15NO2	027489-60-7	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139194.D
Acq On : 27 Aug 2024 18:56
Operator : RC/JU
Sample : P3735-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-13

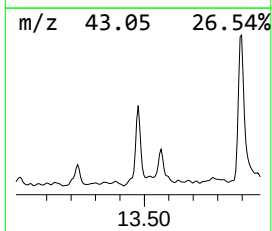
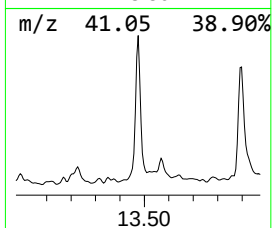
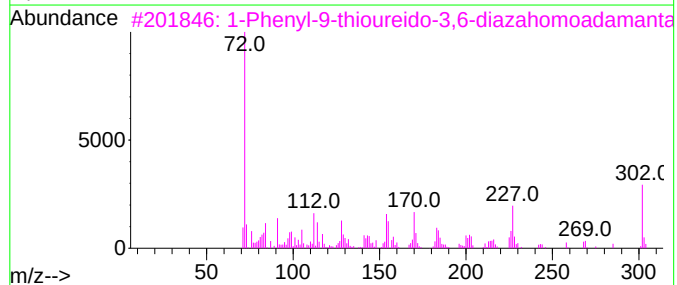
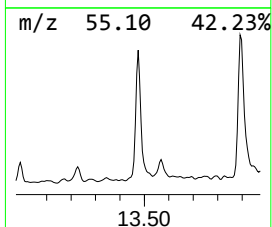
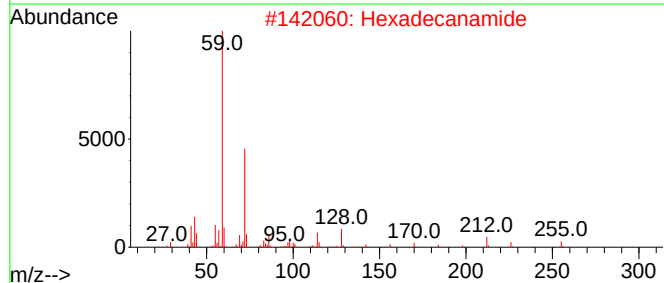
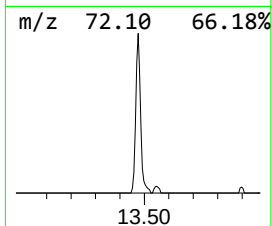
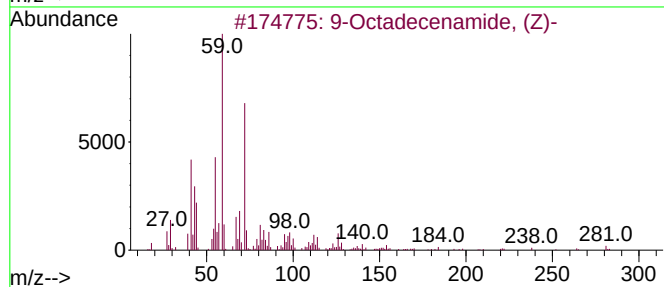
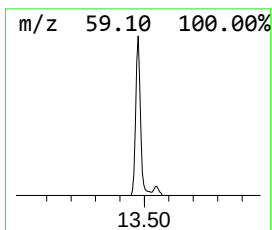
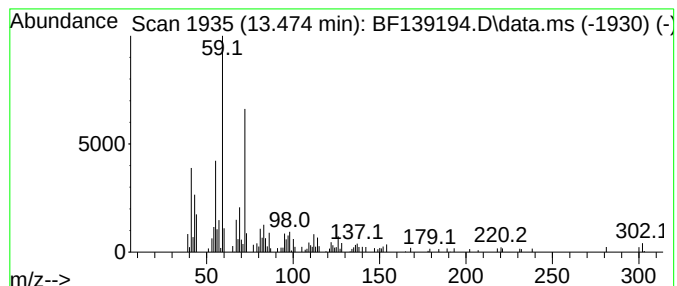
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.474	3.41 ng	107477	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99
2			Hexadecanamide	255	C16H33NO	000629-54-9	72
3			1-Phenyl-9-thioureido-3,6-diazah...	302	C16H22N4S	153464-71-2	53
4			Dodecanamide	199	C12H25NO	001120-16-7	53
5			Octanamide	143	C8H17NO	000629-01-6	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139194.D
Acq On : 27 Aug 2024 18:56
Operator : RC/JU
Sample : P3735-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-13

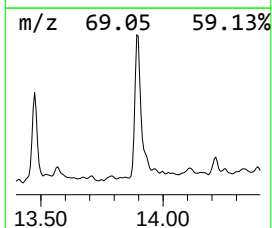
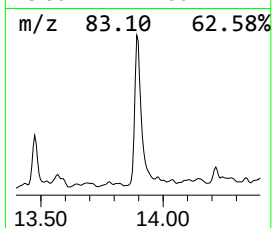
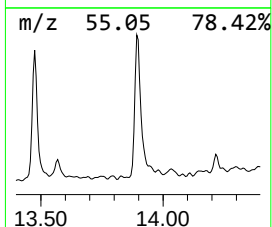
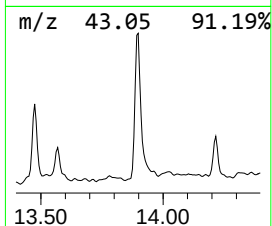
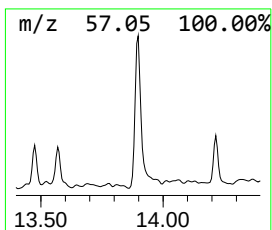
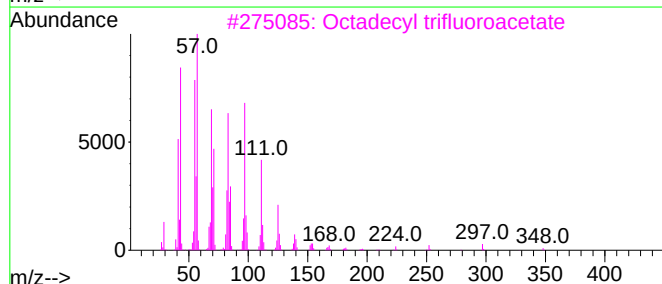
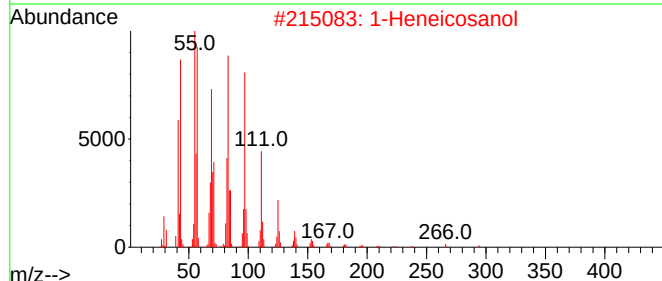
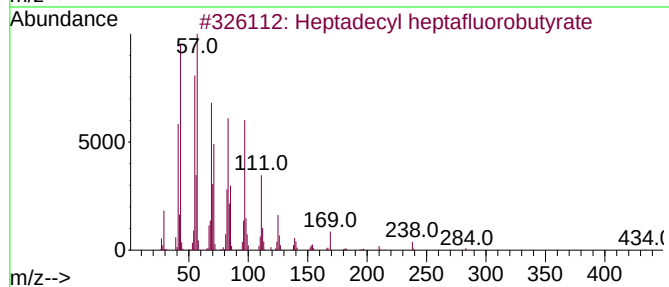
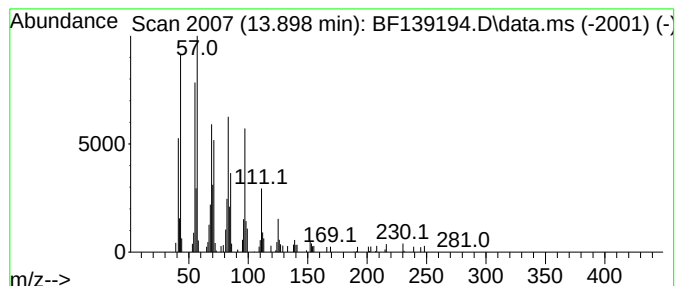
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	3.59 ng	113157	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2			1-Heneicosanol	312	C21H44O	015594-90-8	93
3			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
4			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
5			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139194.D
Acq On : 27 Aug 2024 18:56
Operator : RC/JU
Sample : P3735-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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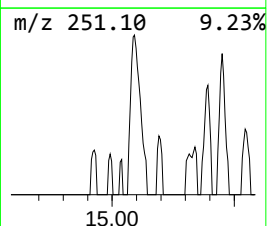
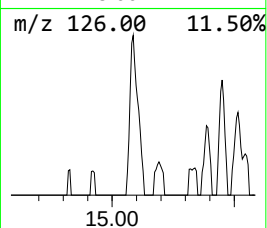
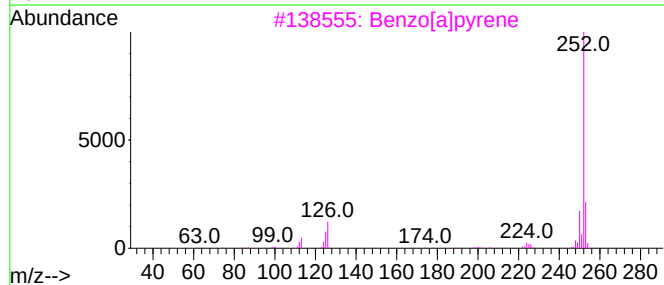
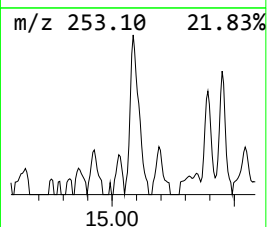
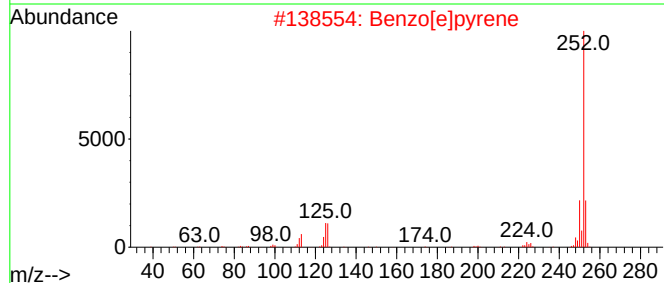
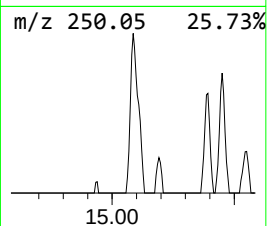
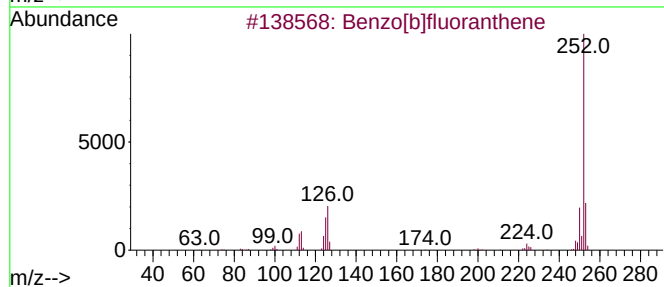
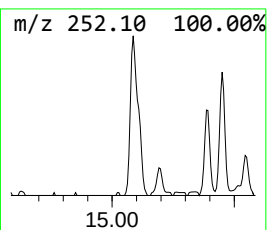
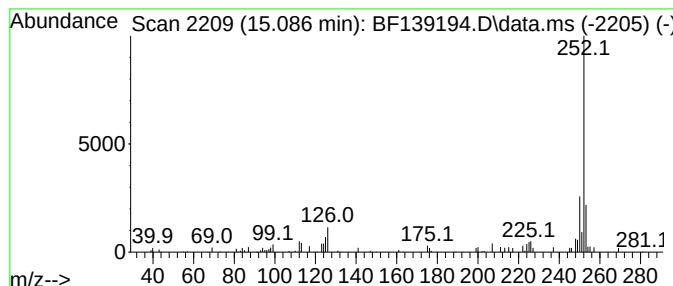
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzo[e]pyrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.086	2.83 ng	56959	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]fluoranthene	252	C20H12	000205-99-2	87
2			Benzo[e]pyrene	252	C20H12	000192-97-2	87
3			Benzo[a]pyrene	252	C20H12	000050-32-8	87
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	87
5			Perylene	252	C20H12	000198-55-0	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139194.D
Acq On : 27 Aug 2024 18:56
Operator : RC/JU
Sample : P3735-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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
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(S)-(+)-1,2-Pro...	3.410	4.3	ng	125045	1	6.892	574776	20.0
2-Pentanone, 4-...	5.116	5.9	ng	168997	1	6.892	574776	20.0
Ethanol, 2-(2-e...	6.710	3.0	ng	84665	1	6.892	574776	20.0
1-Phenoxypropan...	8.480	3.7	ng	132210	2	8.169	708678	20.0
unknown10.016	10.016	5.7	ng	215998	3	9.922	757671	20.0
n-Hexadecanoic ...	11.933	3.4	ng	116138	4	11.410	687244	20.0
9-Octadecenamid...	13.474	3.4	ng	107477	5	14.045	631228	20.0
Heptadecyl hept...	13.898	3.6	ng	113157	5	14.045	631228	20.0
Benzo[e]pyrene	15.086	2.8	ng	56959	6	15.515	403230	20.0