

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080924\
 Data File : BF138896.D
 Acq On : 09 Aug 2024 19:06
 Operator : RC/JU
 Sample : P3509-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OR-02-080724

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-BF073024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138896.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	3	9	21	rVB	658069	1033827	81.28%	10.667%
2	2.252	21	27	36	rBV	8669	13723	1.08%	0.142%
3	3.404	219	223	239	rBV	9097	32229	2.53%	0.333%
4	5.069	500	506	522	rVB	97944	157692	12.40%	1.627%
5	5.475	570	575	597	rVB	926500	1218993	95.84%	12.577%
6	6.487	741	747	767	rBV	928503	1271927	100.00%	13.123%
7	6.681	774	780	791	rBV2	6840	13240	1.04%	0.137%
8	6.839	802	807	812	rBV	235432	282105	22.18%	2.911%
9	7.404	897	903	913	rBV	603876	793329	62.37%	8.185%
10	7.657	941	946	953	rBB	16080	21089	1.66%	0.218%
11	8.122	1016	1025	1037	rVB	277891	360265	28.32%	3.717%
12	8.433	1074	1078	1091	rBV	36882	56109	4.41%	0.579%
13	9.192	1201	1207	1212	rBV	1022047	1255415	98.70%	12.953%
14	9.869	1317	1322	1327	rBV	264371	342279	26.91%	3.532%
15	9.963	1333	1338	1345	rVB2	29235	44790	3.52%	0.462%
16	10.422	1409	1416	1421	rBV	13337	17107	1.34%	0.177%
17	10.663	1452	1457	1469	rBV	368203	475443	37.38%	4.905%
18	10.769	1471	1475	1484	rVB3	8261	14481	1.14%	0.149%
19	11.357	1570	1575	1584	rBV2	221616	361094	28.39%	3.726%
20	11.433	1584	1588	1592	rBV	18184	22567	1.77%	0.233%
21	11.857	1656	1660	1662	rBV	10278	13805	1.09%	0.142%
22	11.886	1662	1665	1670	rVB2	19438	27629	2.17%	0.285%
23	11.969	1676	1679	1688	rVB2	20309	36735	2.89%	0.379%
24	12.410	1749	1754	1756	rBV	12597	18360	1.44%	0.189%
25	12.445	1757	1760	1766	rVB6	12541	20551	1.62%	0.212%
26	12.568	1777	1781	1786	rBV	77457	105505	8.29%	1.089%
27	12.798	1814	1820	1827	rBV	77075	121279	9.54%	1.251%
28	12.939	1838	1844	1849	rBV	712416	885060	69.58%	9.132%
29	13.127	1870	1876	1879	rBV	12741	23026	1.81%	0.238%
30	13.192	1884	1887	1890	rBV	10230	13137	1.03%	0.136%
31	13.363	1912	1916	1919	rBV2	7599	13640	1.07%	0.141%
32	13.845	1993	1998	2007	rBV2	27785	63753	5.01%	0.658%
33	13.998	2019	2024	2036	rVB2	208312	339948	26.73%	3.507%
34	15.462	2268	2273	2289	rVB	125466	221922	17.45%	2.290%

Sum of corrected areas: 9692054

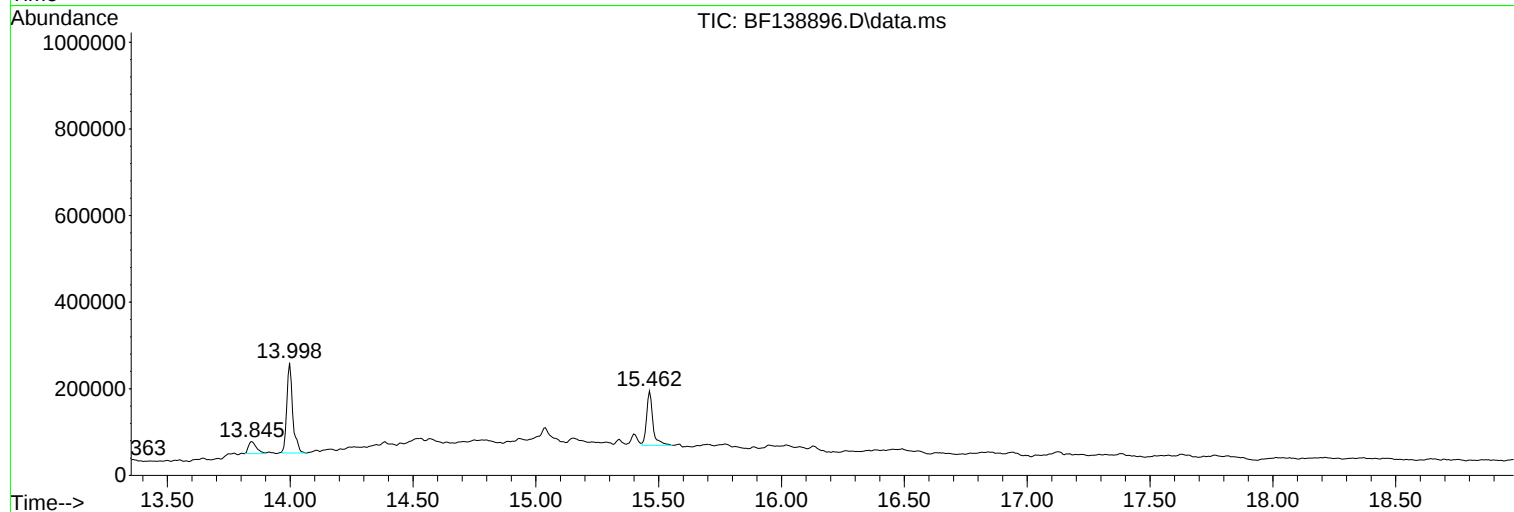
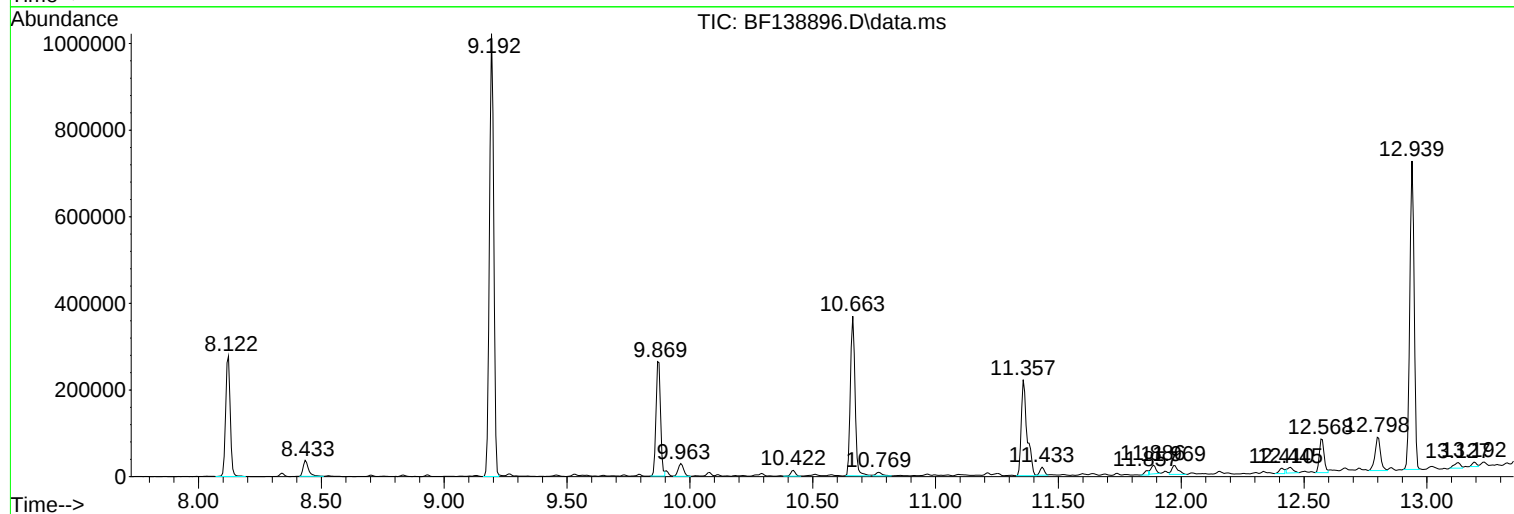
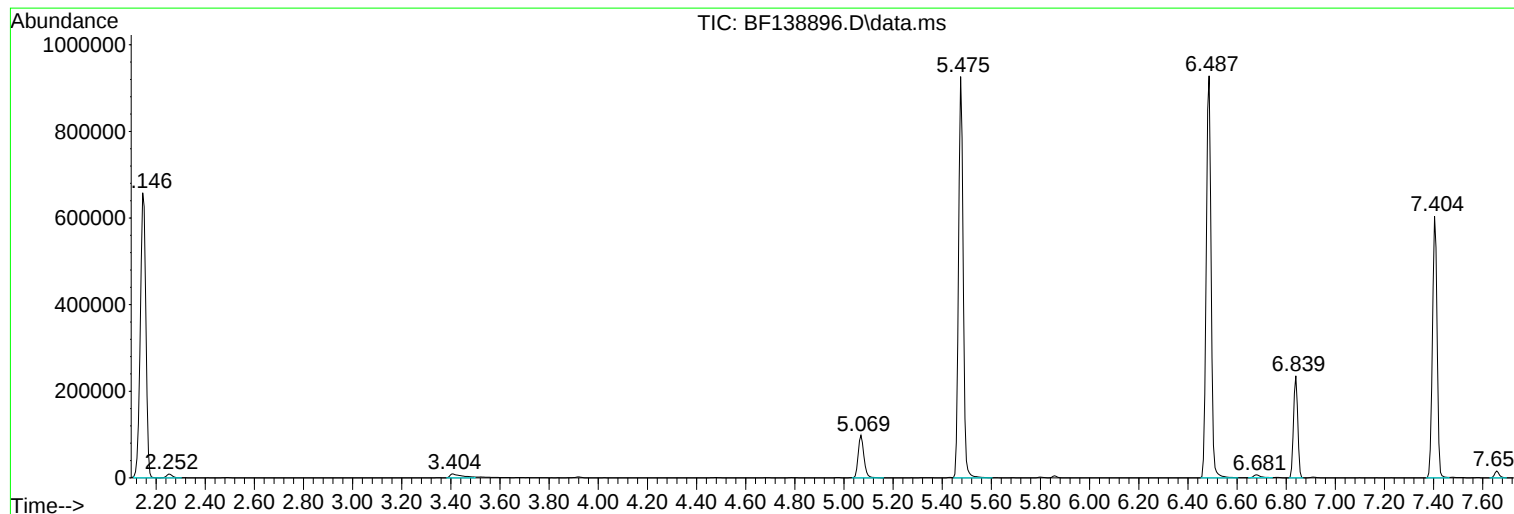
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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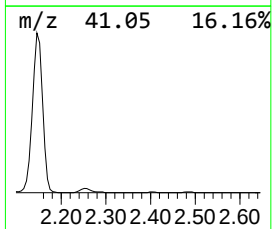
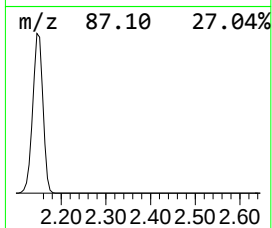
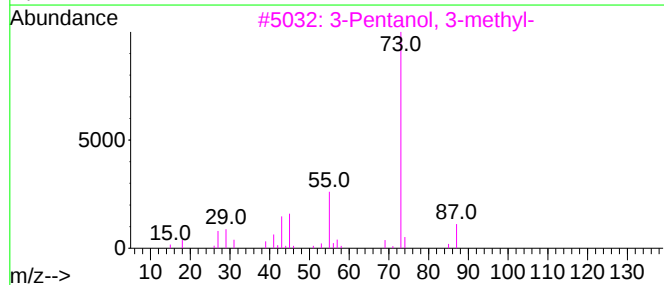
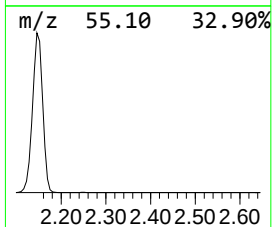
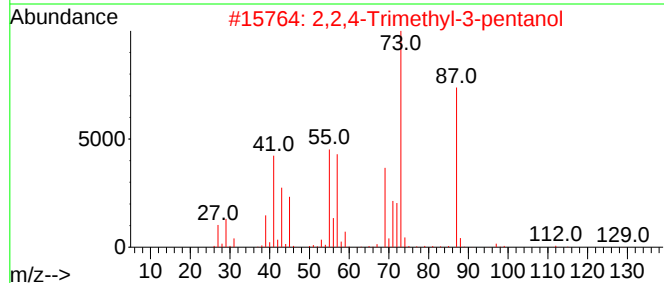
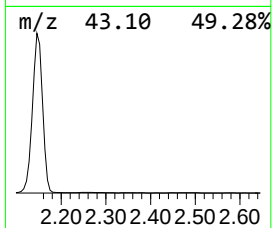
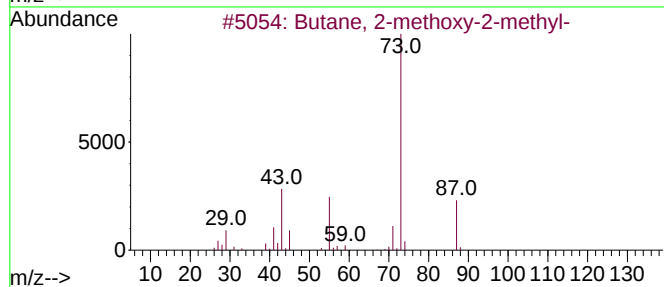
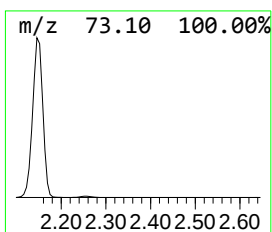
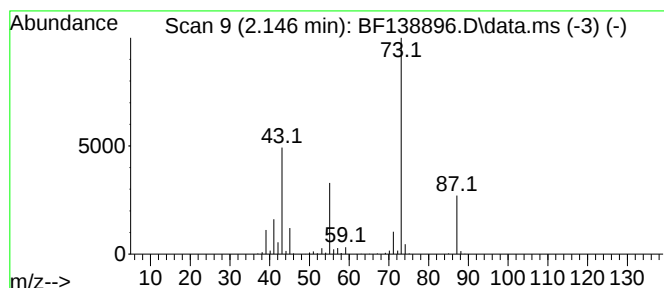
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.146	73.29 ng	1033830	1,4-Dichlorobenzene-d4	6.839

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			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	38
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23



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ClientSampleId :
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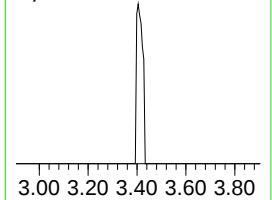
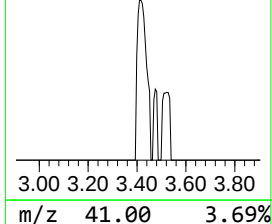
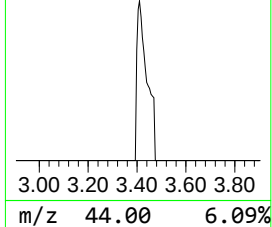
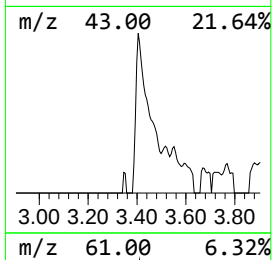
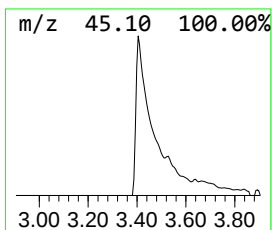
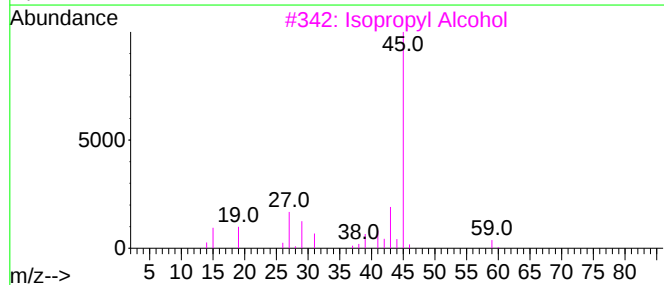
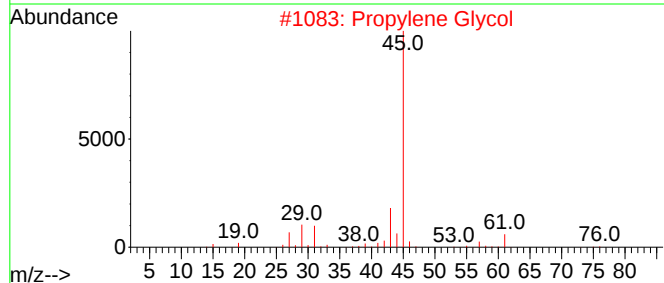
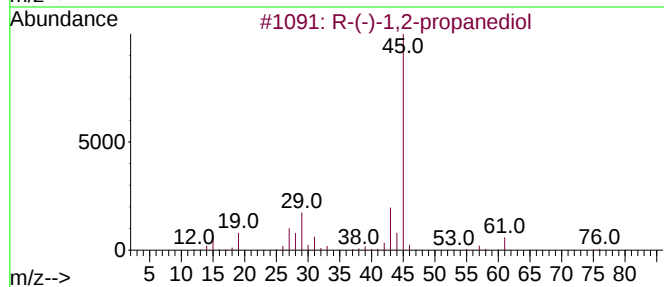
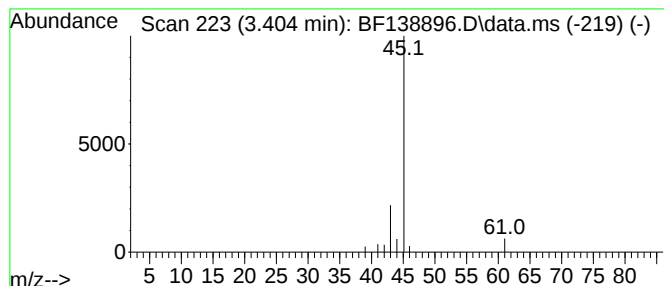
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TIC Integration Parameters: LSCINT.P

Peak Number 2 R-(-)-1,2-propanediol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.404	2.28 ng	32229	1,4-Dichlorobenzene-d4	6.839

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



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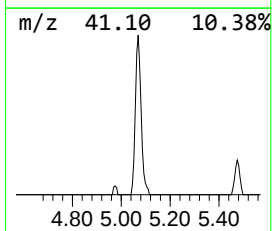
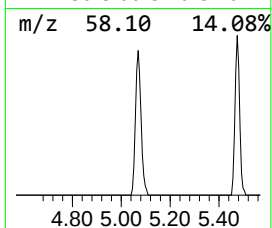
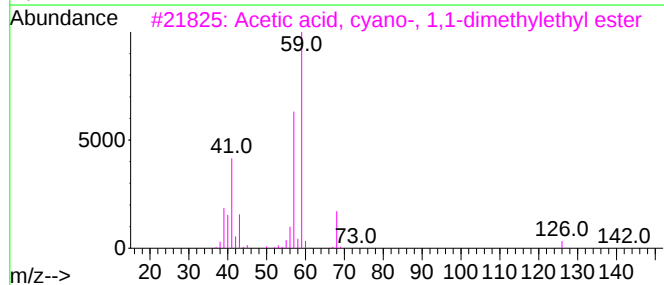
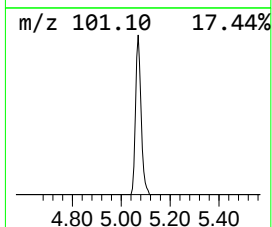
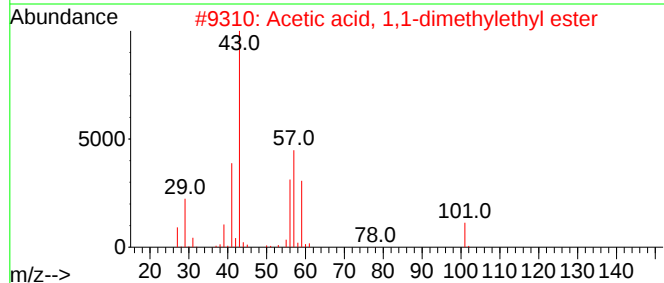
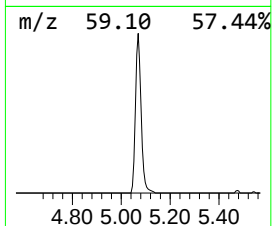
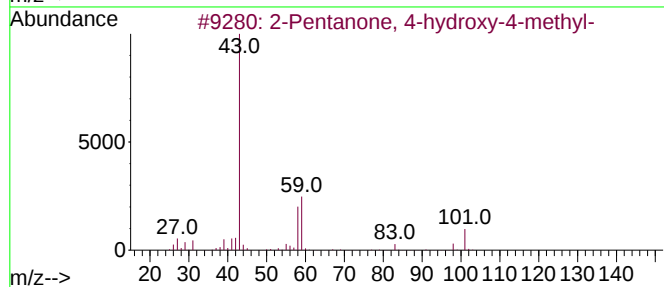
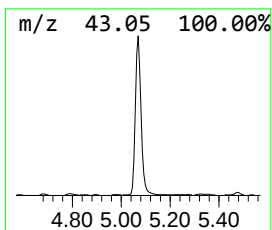
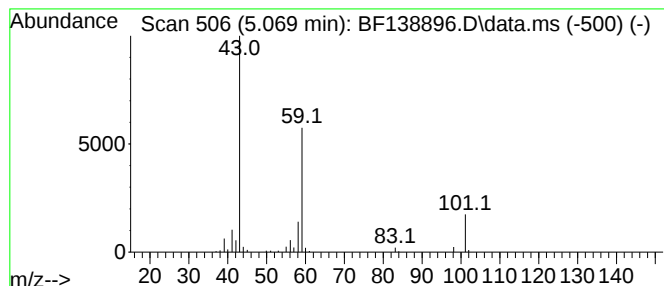
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.069	11.18 ng	157692	1,4-Dichlorobenzene-d4	6.839	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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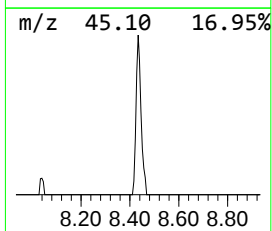
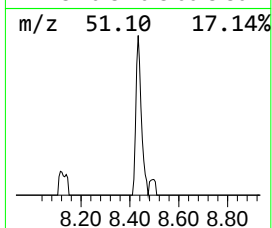
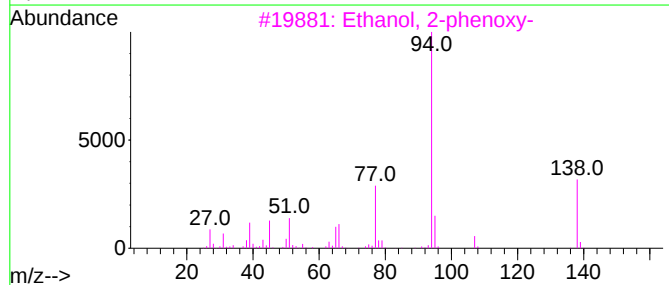
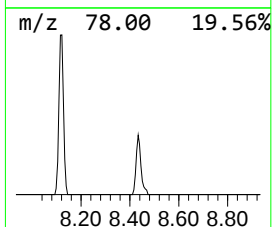
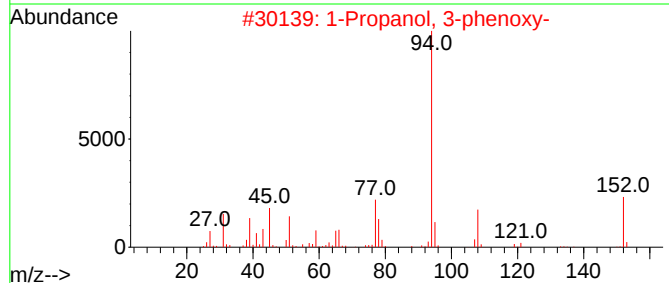
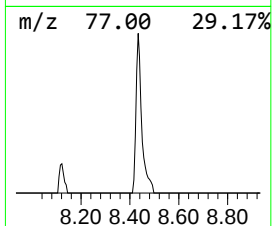
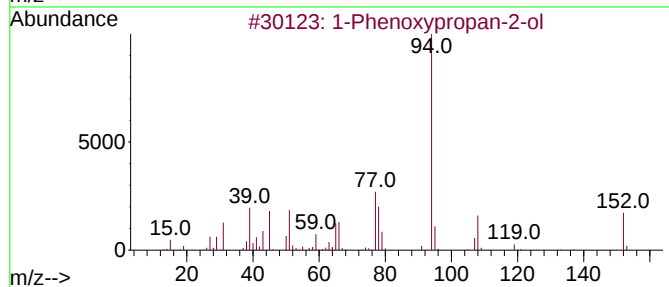
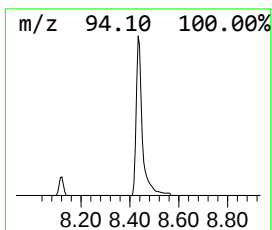
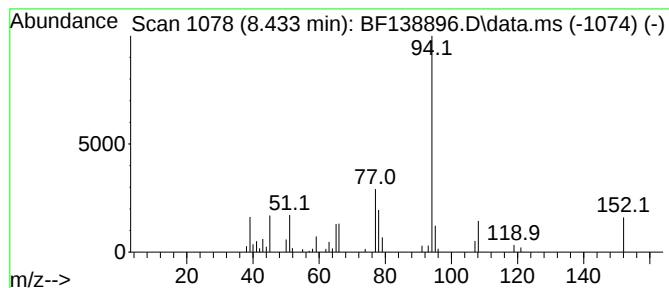
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Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.433	3.11 ng	56109	Naphthalene-d8	8.122

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	72
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	59
4			Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	53
5			3-(.alpha.-Hydroxyethyl)-aniline	137	C8H11NO	002454-37-7	53



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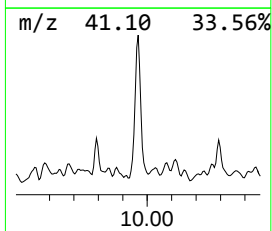
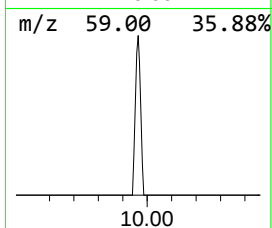
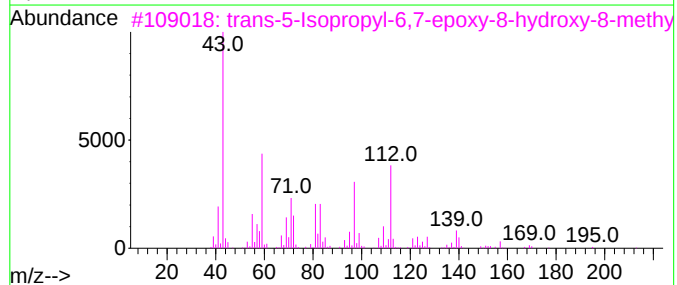
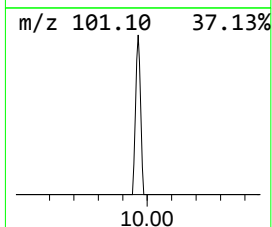
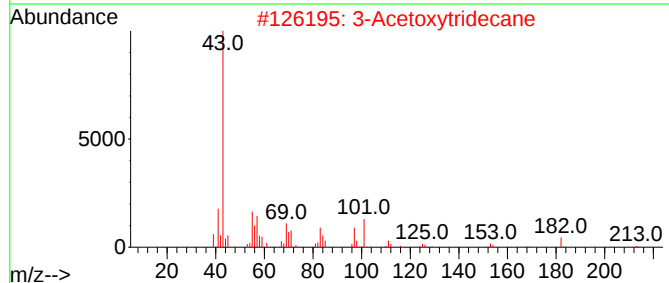
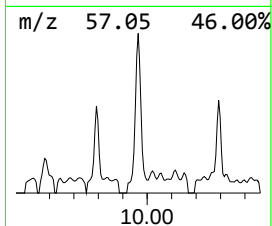
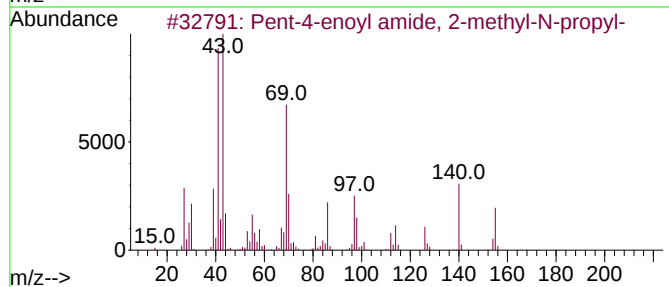
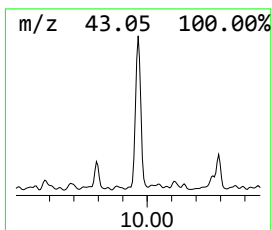
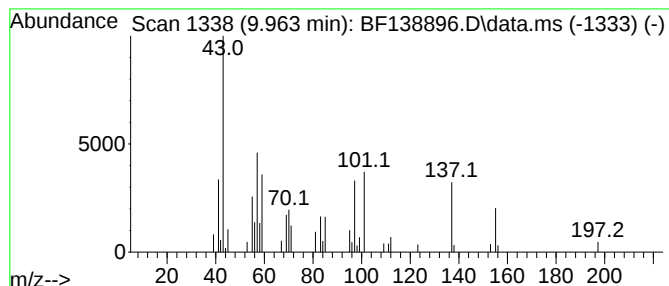
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown9.963 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.963	2.62 ng	44790	Acenaphthene-d10	9.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pent-4-enoyl amide, 2-methyl-N-p...	155	C9H17NO	1000420-35-2	22
2			3-Acetoxytridecane	242	C15H30O2	1010245-61-3	12
3			trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	12
4			3-Octanol, acetate	172	C10H20O2	004864-61-3	10
5			Decanoic acid, 2-propenyl ester	212	C13H24O2	057856-81-2	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080924\
Data File : BF138896.D
Acq On : 09 Aug 2024 19:06
Operator : RC/JU
Sample : P3509-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-02-080724

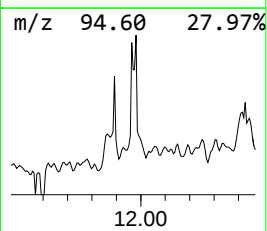
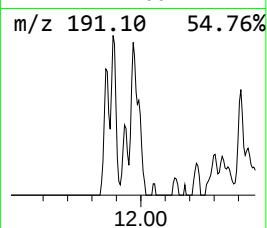
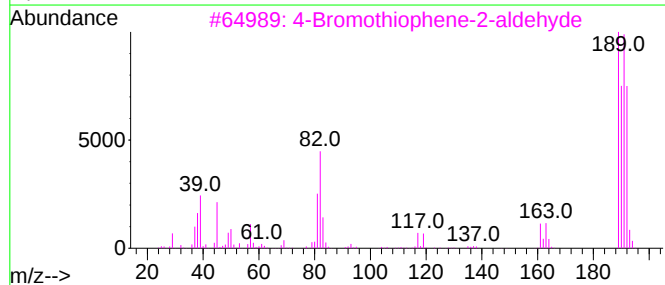
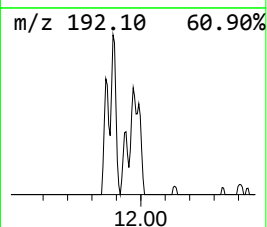
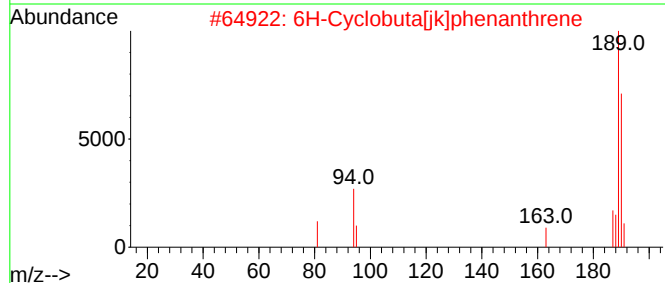
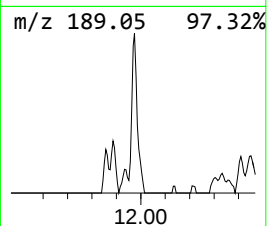
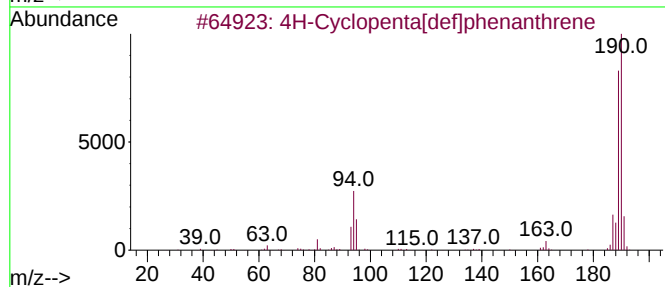
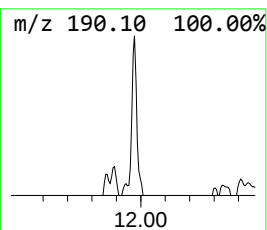
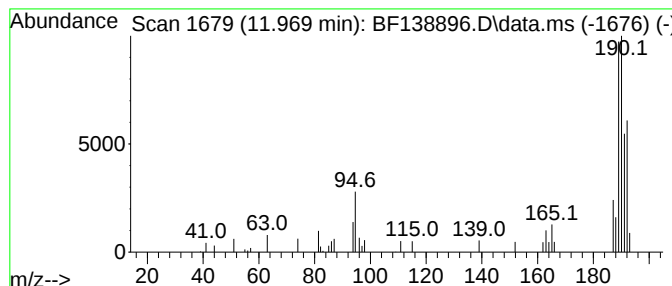
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.969	2.03 ng	36735	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	50
2			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
3			4-Bromothiophene-2-aldehyde	190	C5H3BrOS	018791-75-8	38
4			1H-Pyrazole-4-carboxaldehyde, 1-...	190	C10H7FN2O	1000338-05-6	32
5			Propyne, 1,3-diphenyl-	192	C15H12	004980-70-5	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080924\
Data File : BF138896.D
Acq On : 09 Aug 2024 19:06
Operator : RC/JU
Sample : P3509-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-02-080724

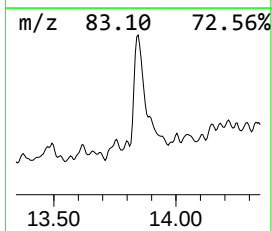
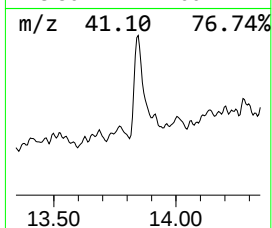
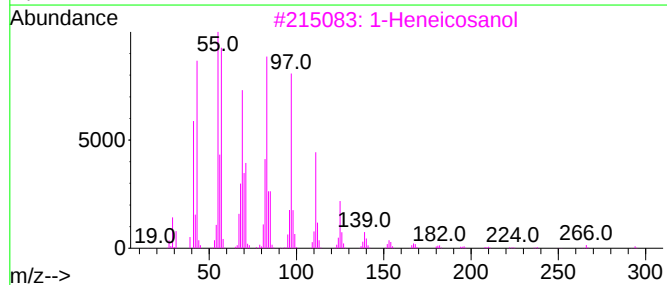
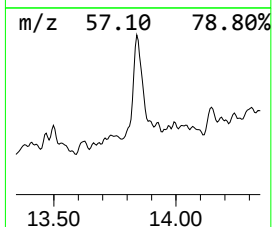
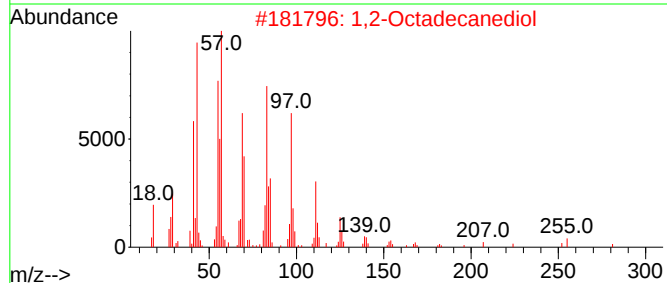
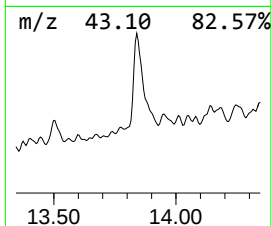
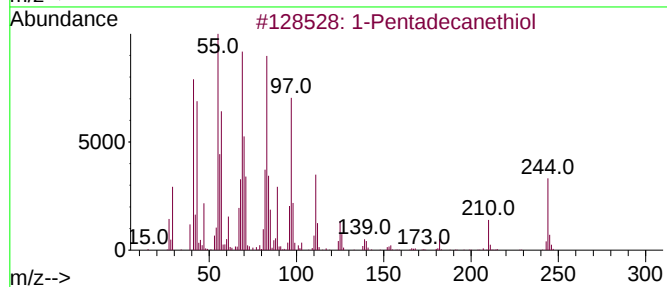
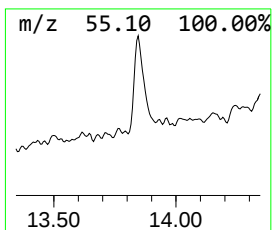
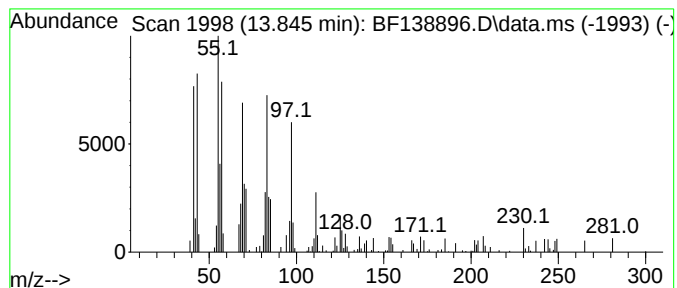
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Pentadecanethiol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	3.75 ng	63753	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentadecanethiol	244	C15H32S	025276-70-4	95
2			1,2-Octadecanediol	286	C18H38O2	020294-76-2	87
3			1-Heneicosanol	312	C21H44O	015594-90-8	87
4			1-Tricosene	322	C23H46	018835-32-0	81
5			1-Octadecanol	270	C18H38O	000112-92-5	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080924\
Data File : BF138896.D
Acq On : 09 Aug 2024 19:06
Operator : RC/JU
Sample : P3509-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-02-080724

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.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...	2.146	73.3	ng	1033830	1	6.839	282105	20.0
R-(-)-1,2-propa...	3.404	2.3	ng	32229	1	6.839	282105	20.0
2-Pentanone, 4-...	5.069	11.2	ng	157692	1	6.839	282105	20.0
1-Phenoxypropan...	8.433	3.1	ng	56109	2	8.122	360265	20.0
unknown9.963	9.963	2.6	ng	44790	3	9.875	342279	20.0
4H-Cyclopenta[d...	11.969	2.0	ng	36735	4	11.357	361094	20.0
1-Pentadecanethiol	13.845	3.8	ng	63753	5	13.998	339948	20.0