

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080324\
 Data File : BF138771.D
 Acq On : 03 Aug 2024 15:43
 Operator : RC/JU
 Sample : P3448-11
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP6

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: BF138771.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	7	21	rVB	768564	1170097	82.99%	8.853%
2	3.381	215	219	232	rBV	11178	30553	2.17%	0.231%
3	5.069	500	506	516	rVB	63548	95831	6.80%	0.725%
4	5.475	570	575	593	rBV	951130	1246809	88.43%	9.434%
5	6.487	741	747	767	rVB	989482	1310762	92.97%	9.918%
6	6.675	775	779	789	rBV2	13710	21958	1.56%	0.166%
7	6.846	803	808	813	rVB	288176	358631	25.44%	2.714%
8	7.410	897	904	912	rBV	616121	831918	59.00%	6.295%
9	7.657	942	946	952	rVB	24682	31297	2.22%	0.237%
10	8.122	1020	1025	1033	rVB	393387	501301	35.56%	3.793%
11	8.440	1074	1079	1092	rBV	45562	72905	5.17%	0.552%
12	9.198	1202	1208	1213	rBV	1132989	1409927	100.00%	10.668%
13	9.875	1318	1323	1333	rVV	447544	584872	41.48%	4.425%
14	9.969	1334	1339	1346	rVB	34935	53048	3.76%	0.401%
15	10.669	1452	1458	1472	rBV	610913	797793	56.58%	6.036%
16	10.781	1472	1477	1486	rVB2	14257	28019	1.99%	0.212%
17	11.363	1571	1576	1586	rBV	370501	525130	37.25%	3.973%
18	11.439	1586	1589	1593	rVB	12725	14945	1.06%	0.113%
19	11.892	1657	1666	1672	rBV3	38713	71978	5.11%	0.545%
20	11.980	1677	1681	1690	rVB4	15138	30241	2.14%	0.229%
21	12.063	1690	1695	1700	rBV6	8684	18871	1.34%	0.143%
22	12.580	1778	1783	1788	rBV	118404	154745	10.98%	1.171%
23	12.810	1815	1822	1835	rVB	131658	219675	15.58%	1.662%
24	12.951	1840	1846	1853	rVB	878987	1160708	82.32%	8.782%
25	13.027	1853	1859	1866	rBV4	13946	27463	1.95%	0.208%
26	13.127	1869	1876	1880	rBV3	26426	51124	3.63%	0.387%
27	13.239	1891	1895	1902	rVB3	12714	28611	2.03%	0.216%
28	13.327	1907	1910	1914	rVV2	19644	28508	2.02%	0.216%
29	13.510	1938	1941	1951	rBV10	7331	17591	1.25%	0.133%
30	13.851	1995	1999	2010	rVB2	48921	104568	7.42%	0.791%
31	14.004	2017	2025	2039	rBV2	286698	519259	36.83%	3.929%
32	14.110	2039	2043	2049	rBV	26321	39726	2.82%	0.301%
33	14.392	2082	2091	2094	rBV	18440	39642	2.81%	0.300%
34	14.469	2101	2104	2106	rBV3	10595	15002	1.06%	0.114%
35	14.580	2119	2123	2128	rVB4	8598	19381	1.37%	0.147%
36	14.886	2172	2175	2181	rVB5	13283	22392	1.59%	0.169%

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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
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37	15.045	2197	2202	2211	rBV	188076	401120	28.45%	3.035%
38	15.151	2217	2220	2231	rVB	38339	62941	4.46%	0.476%
39	15.351	2249	2254	2259	rVB	111759	171696	12.18%	1.299%
40	15.410	2259	2264	2269	rVV	121113	176995	12.55%	1.339%
41	15.474	2269	2275	2290	rVB2	276266	507070	35.96%	3.837%
42	15.992	2360	2363	2367	rBV7	10492	20249	1.44%	0.153%
43	16.939	2518	2524	2531	rBV2	56640	127124	9.02%	0.962%
44	17.386	2594	2600	2611	rVB	40728	93902	6.66%	0.710%

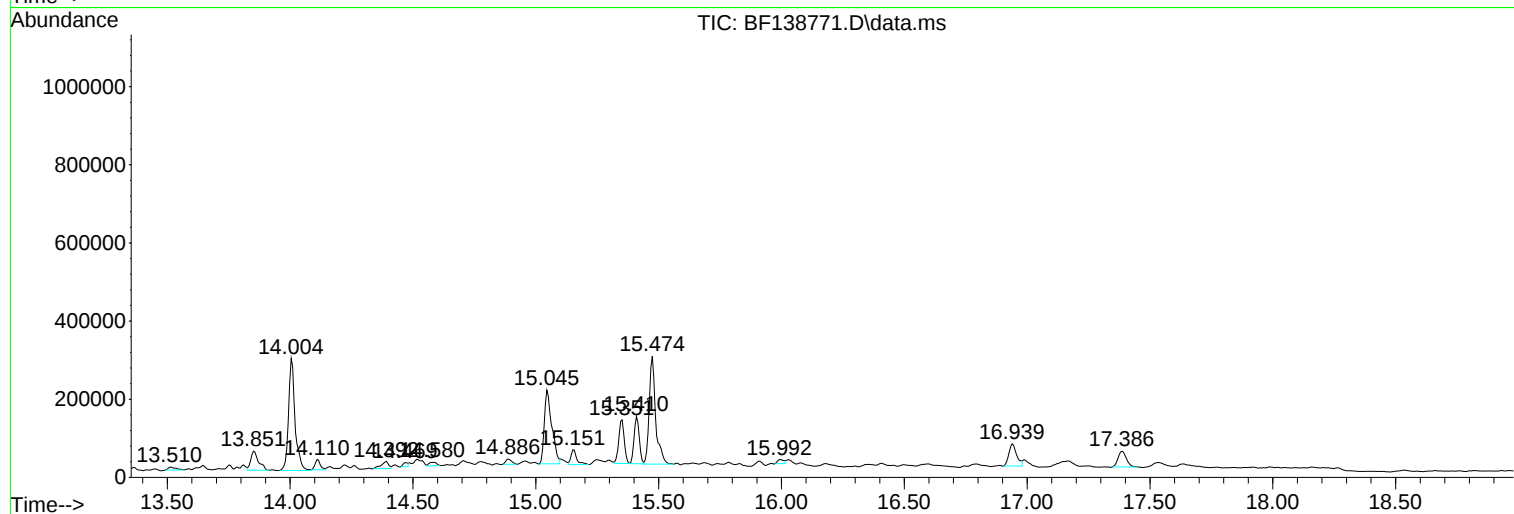
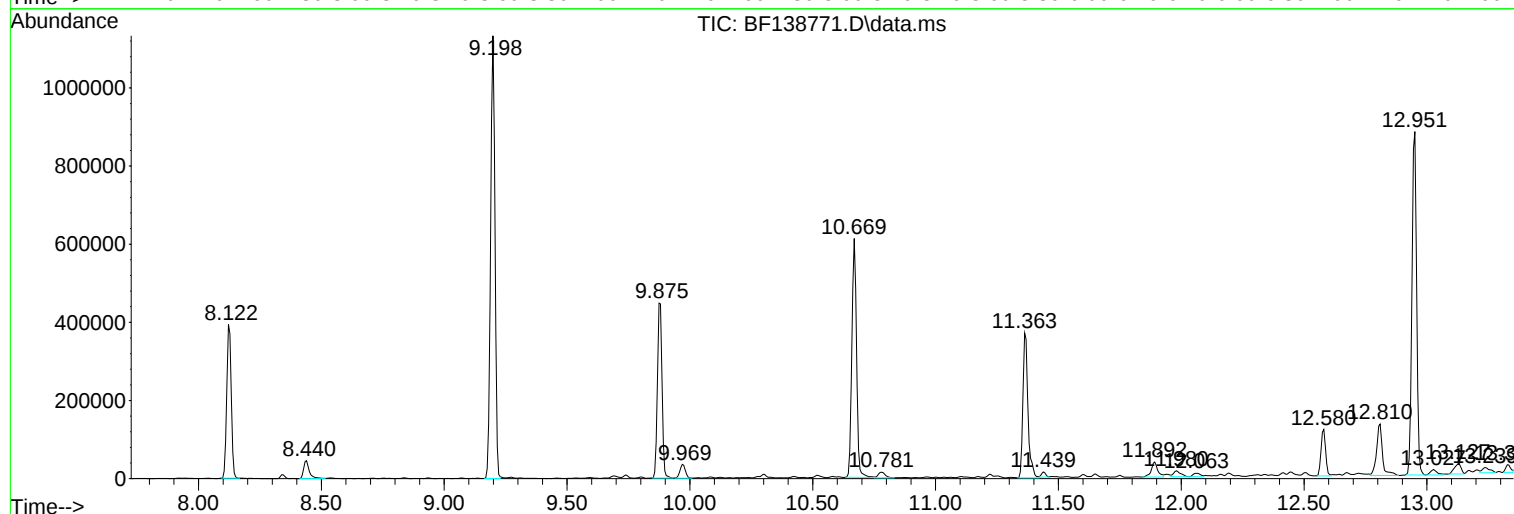
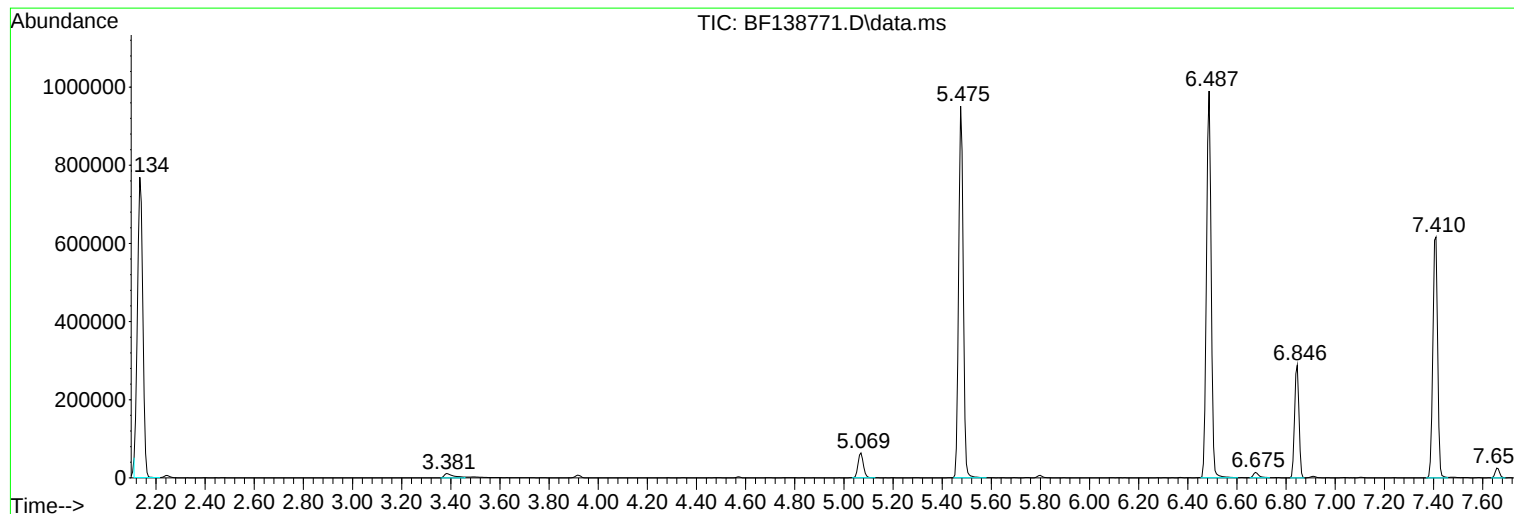
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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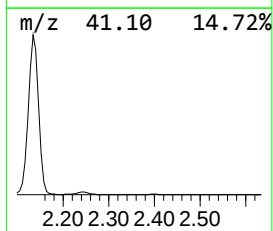
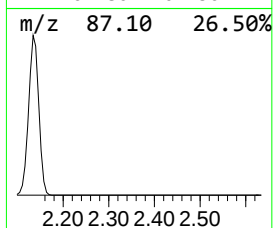
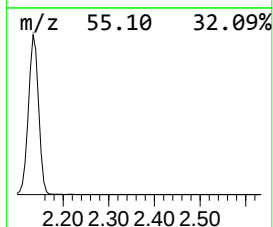
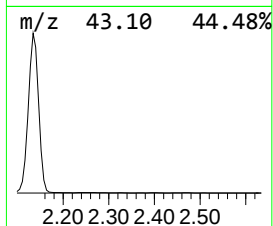
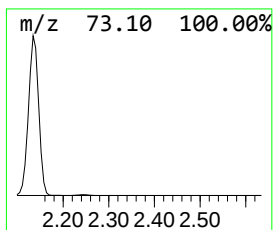
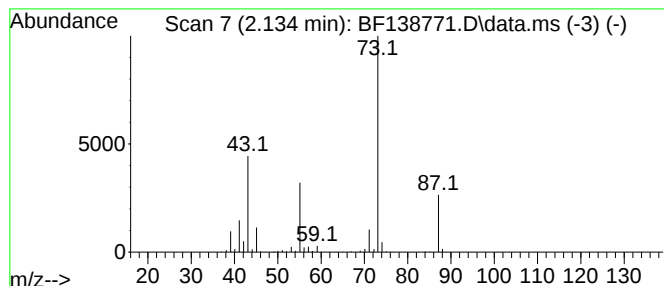
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	65.25 ng	1170100	1,4-Dichlorobenzene-d4	6.846

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	23
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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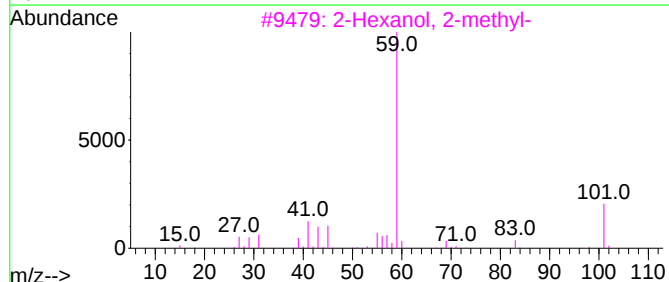
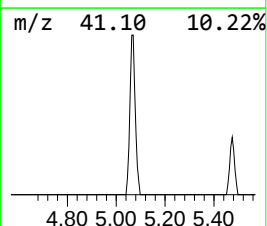
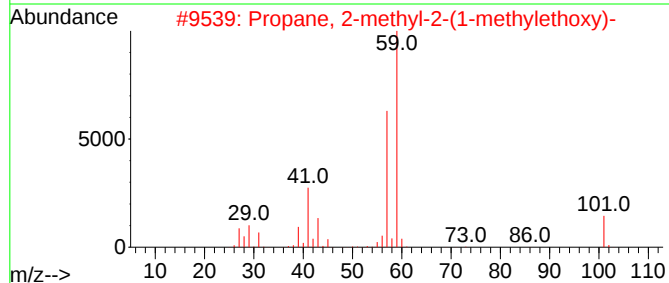
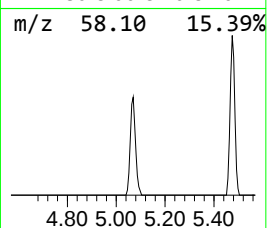
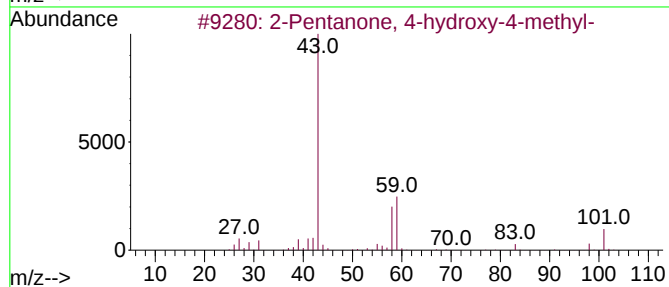
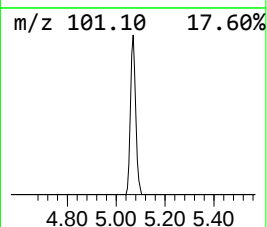
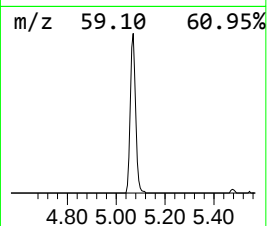
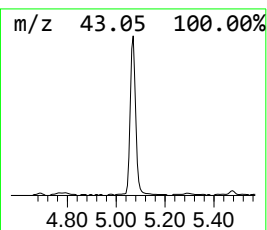
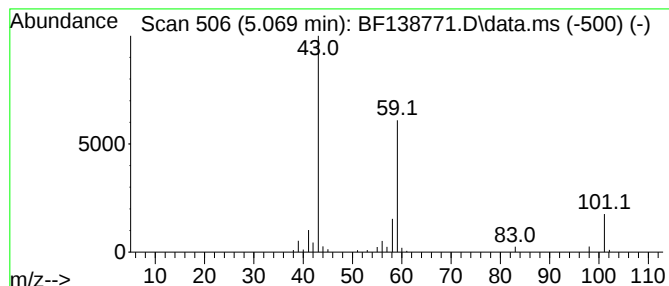
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.069	5.34 ng	95831	1,4-Dichlorobenzene-d4	6.846

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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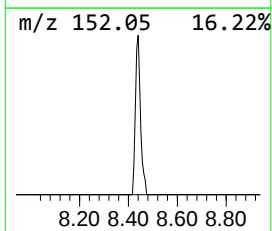
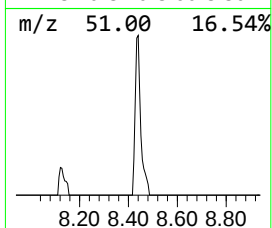
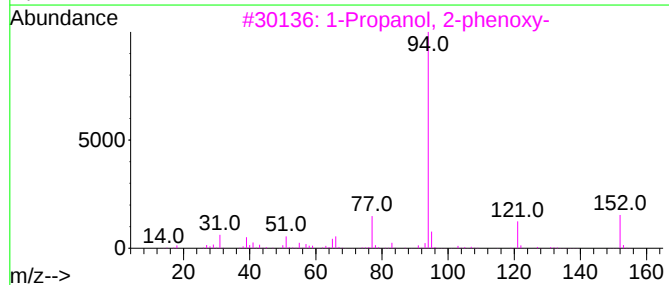
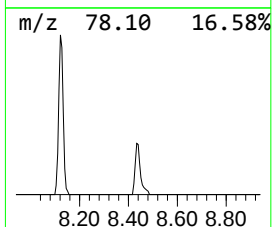
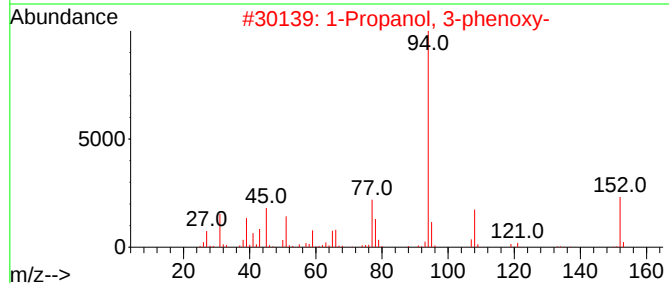
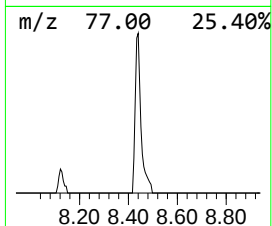
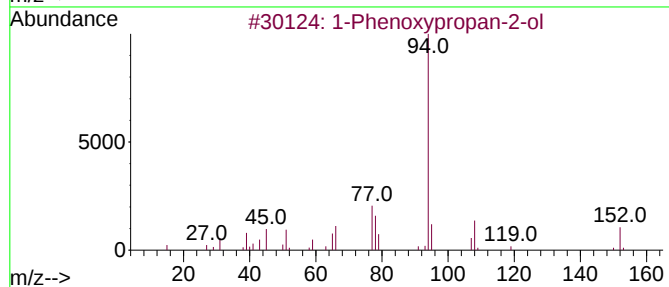
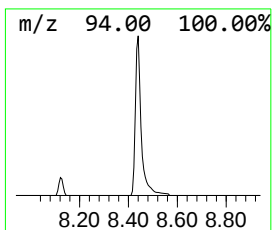
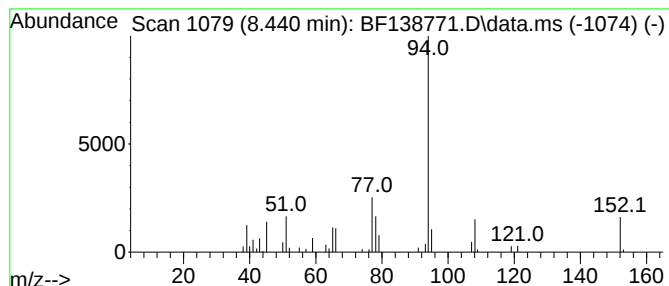
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.440	2.91 ng	72905	Naphthalene-d8	8.122

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
2		1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	91
3		1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59
4		Benzene, propoxy-	136	C9H12O	000622-85-5	53
5		Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	53



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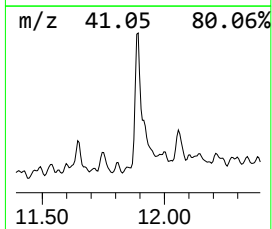
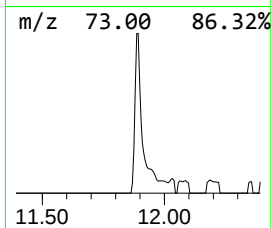
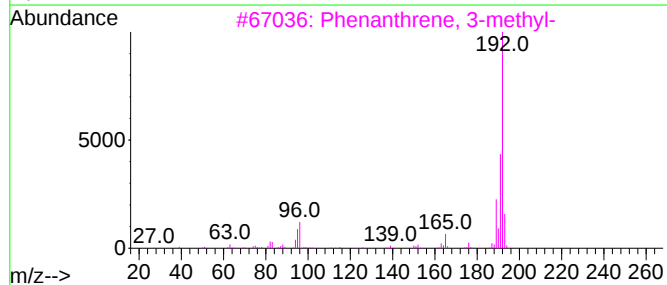
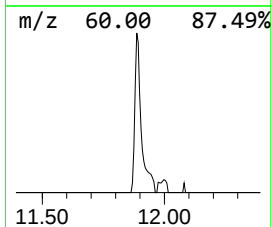
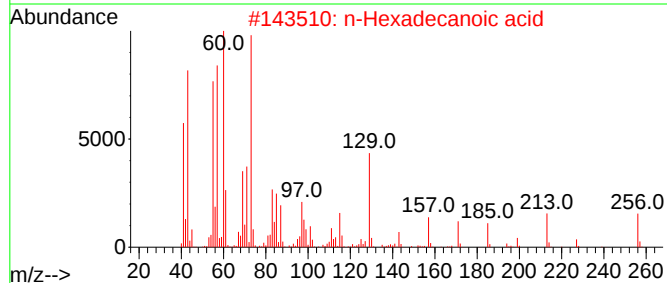
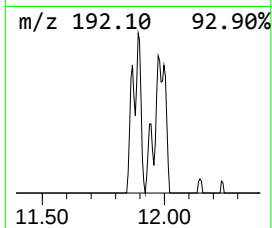
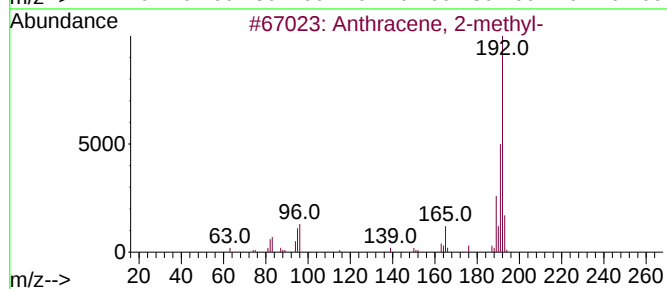
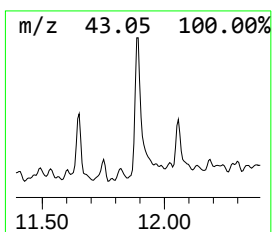
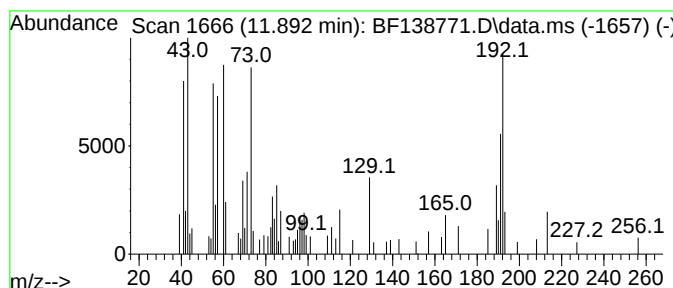
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Anthracene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	2.74 ng	71978	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 2-methyl-	192	C15H12	000613-12-7	50
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	47
3			Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	42
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	41
5			Anthracene, 1-methyl-	192	C15H12	000610-48-0	38



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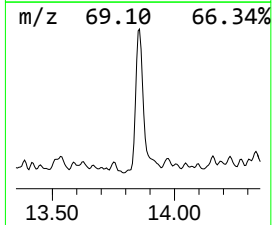
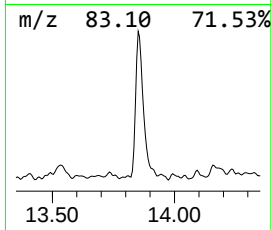
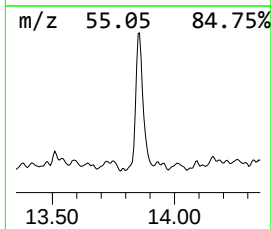
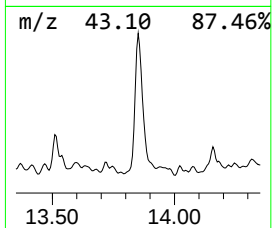
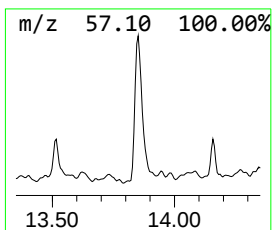
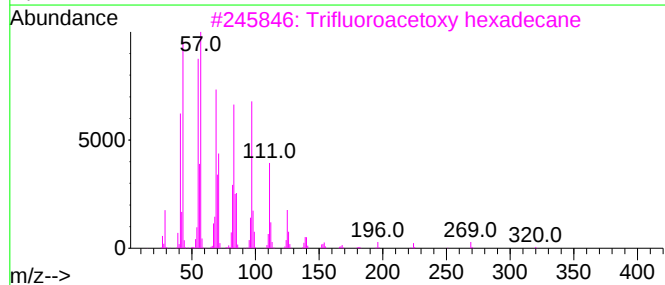
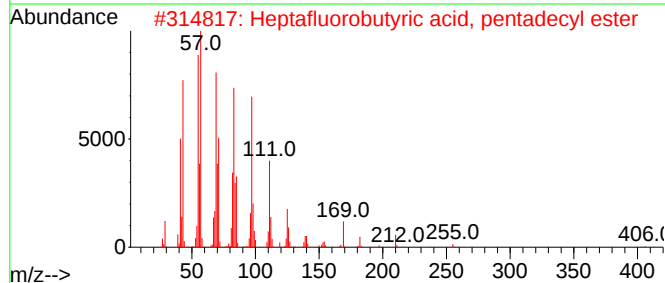
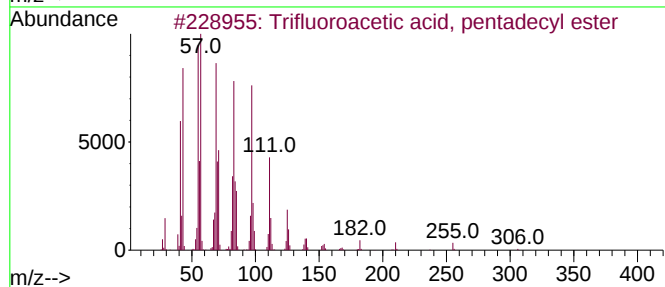
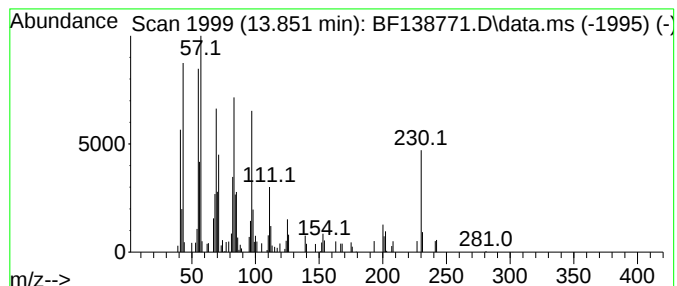
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Trifluoroacetic acid, penta... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.851	4.03 ng	104568	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
2			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
4			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
5			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080324\
Data File : BF138771.D
Acq On : 03 Aug 2024 15:43
Operator : RC/JU
Sample : P3448-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP6

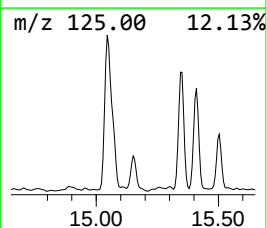
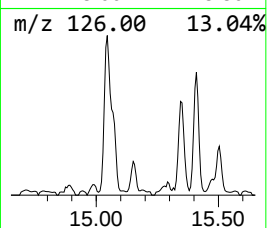
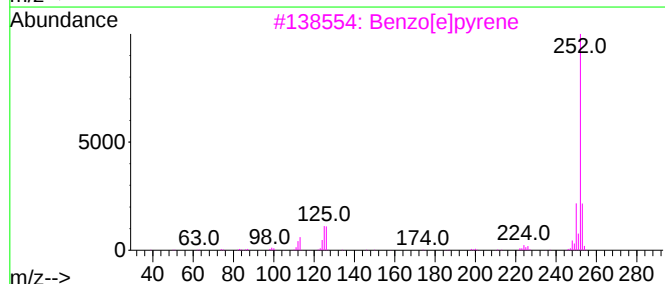
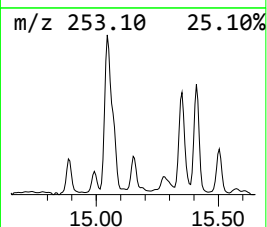
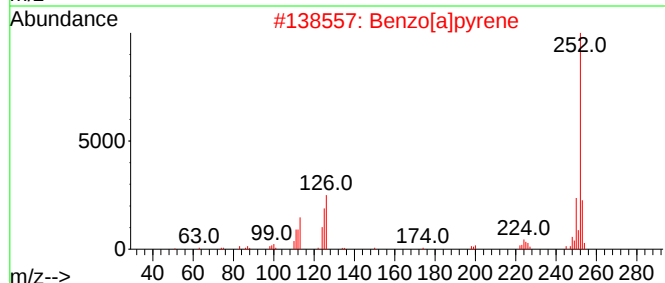
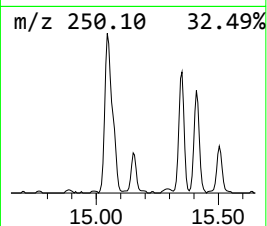
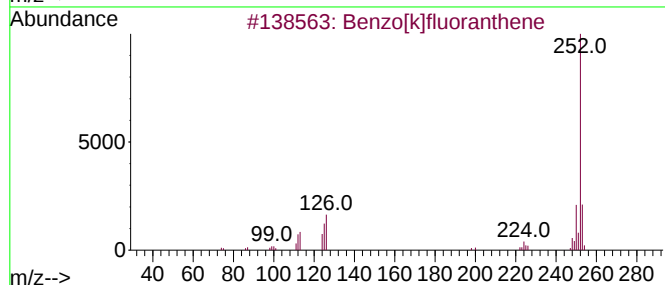
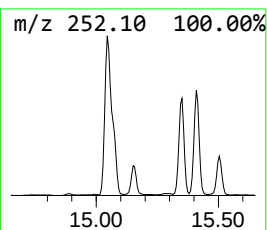
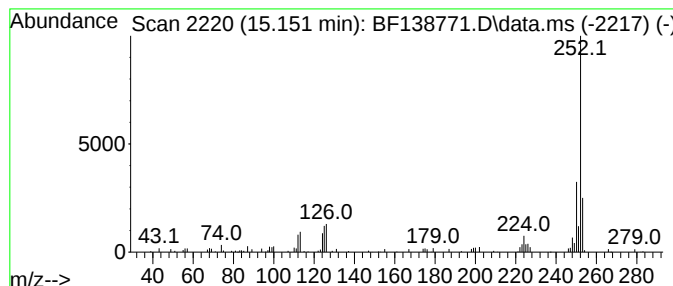
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.151	2.48 ng	62941	Perylene-d12	15.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
2			Benzo[a]pyrene	252	C20H12	000050-32-8	91
3			Benzo[e]pyrene	252	C20H12	000192-97-2	91
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	90
5			Perylene	252	C20H12	000198-55-0	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080324\
Data File : BF138771.D
Acq On : 03 Aug 2024 15:43
Operator : RC/JU
Sample : P3448-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP6

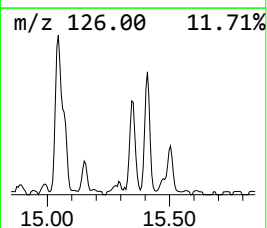
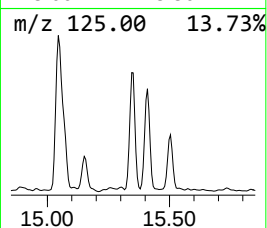
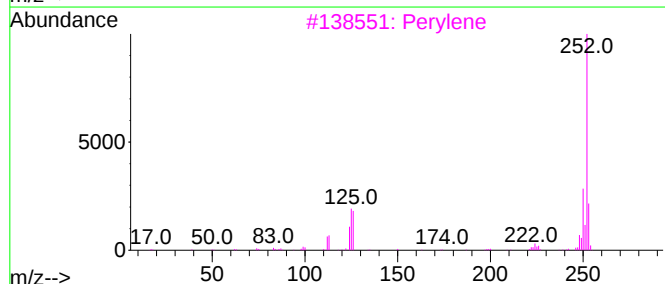
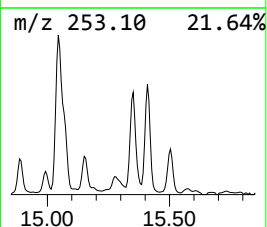
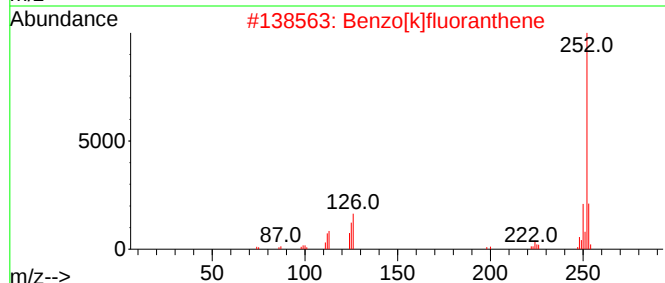
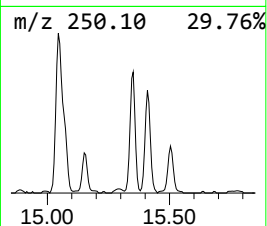
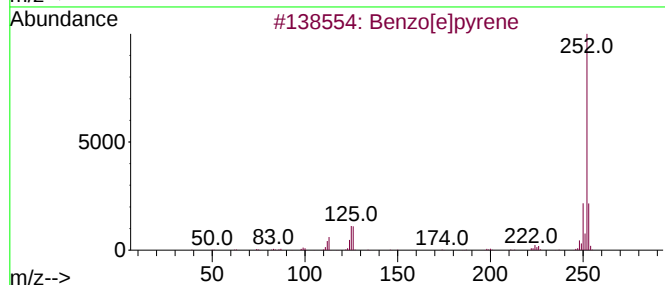
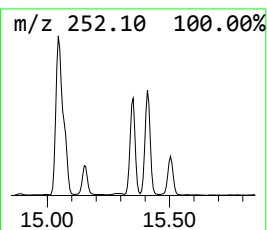
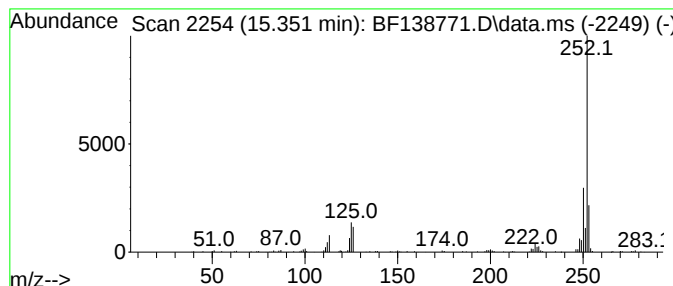
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Perylene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.351	6.77 ng	171696	Perylene-d12	15.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3			Perylene	252	C20H12	000198-55-0	97
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080324\
Data File : BF138771.D
Acq On : 03 Aug 2024 15:43
Operator : RC/JU
Sample : P3448-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP6

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...	2.134	65.3	ng	1170100	1	6.846	358631	20.0
2-Pentanone, 4-...	5.069	5.3	ng	95831	1	6.846	358631	20.0
1-Phenoxypropan...	8.440	2.9	ng	72905	2	8.122	501301	20.0
Anthracene, 2-m...	11.892	2.7	ng	71978	4	11.363	525130	20.0
Trifluoroacetic...	13.851	4.0	ng	104568	5	14.004	519259	20.0
Benzo[e]pyrene	15.151	2.5	ng	62941	6	15.474	507070	20.0
Perylene	15.351	6.8	ng	171696	6	15.474	507070	20.0