

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
 Data File : BF139195.D
 Acq On : 27 Aug 2024 19:26
 Operator : RC/JU
 Sample : P3735-13
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-16

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: BF139195.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	9	16	23	rVB	728331	1108813	80.00%	7.600%
2	3.393	217	221	237	rBV	5462	17421	1.26%	0.119%
3	5.098	503	511	524	rBV	58380	92162	6.65%	0.632%
4	5.504	574	580	585	rBV	1001163	1270037	91.63%	8.705%
5	6.510	745	751	756	rBV	1020407	1313968	94.80%	9.006%
6	6.710	780	785	800	rBV	31286	42435	3.06%	0.291%
7	6.892	810	816	821	rBV	428689	535847	38.66%	3.673%
8	7.451	905	911	916	rBV	624617	806789	58.21%	5.530%
9	7.704	948	954	958	rBV	12412	14213	1.03%	0.097%
10	8.169	1028	1033	1041	rBV	530894	677151	48.86%	4.641%
11	8.481	1081	1086	1096	rVB	52624	68259	4.92%	0.468%
12	9.245	1210	1216	1221	rBV	1135865	1386015	100.00%	9.499%
13	9.581	1268	1273	1276	rBV	13288	17828	1.29%	0.122%
14	9.781	1303	1307	1314	rVB	16231	20186	1.46%	0.138%
15	9.922	1326	1331	1336	rBV	584991	714493	51.55%	4.897%
16	10.016	1342	1347	1353	rBV	86048	128206	9.25%	0.879%
17	10.128	1361	1366	1369	rBV	12547	15770	1.14%	0.108%
18	10.469	1420	1424	1430	rVB	22475	27937	2.02%	0.191%
19	10.704	1459	1464	1479	rBV	560917	736747	53.16%	5.049%
20	11.016	1511	1517	1520	rBV3	8972	14978	1.08%	0.103%
21	11.304	1563	1566	1571	rVB	15330	18391	1.33%	0.126%
22	11.410	1579	1584	1592	rBV2	465273	810603	58.48%	5.556%
23	11.480	1592	1596	1600	rVV	24662	30089	2.17%	0.206%
24	11.633	1617	1622	1631	rBV2	11180	22709	1.64%	0.156%
25	11.739	1637	1640	1644	rVB3	12213	15114	1.09%	0.104%
26	11.804	1645	1651	1658	rVB3	12011	24893	1.80%	0.171%
27	11.910	1664	1669	1670	rBV	36524	42887	3.09%	0.294%
28	11.933	1670	1673	1678	rVV2	65241	88224	6.37%	0.605%
29	11.980	1678	1681	1684	rVV2	10731	14588	1.05%	0.100%
30	12.022	1684	1688	1696	rVB	52848	103883	7.50%	0.712%
31	12.204	1715	1719	1730	rVB4	24022	51401	3.71%	0.352%
32	12.457	1758	1762	1765	rBV	33702	45098	3.25%	0.309%
33	12.492	1765	1768	1774	rVV3	22073	47804	3.45%	0.328%
34	12.545	1774	1777	1781	rVV4	18114	26621	1.92%	0.182%
35	12.622	1785	1790	1794	rVB	215952	278694	20.11%	1.910%
36	12.845	1821	1828	1834	rBV	204932	309158	22.31%	2.119%

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37	12.898	1834	1837	1842	rVB3	16199	23894	1.72%	0.164%
38	12.992	1842	1853	1860	rVB	865641	1101898	79.50%	7.552%
39	13.063	1860	1865	1872	rBV4	28208	57483	4.15%	0.394%
40	13.174	1876	1884	1888	rVB2	41508	84336	6.08%	0.578%
41	13.239	1888	1895	1898	rBV4	28327	47568	3.43%	0.326%
42	13.280	1898	1902	1909	rVB	35879	50043	3.61%	0.343%
43	13.369	1913	1917	1920	rBV	21658	27158	1.96%	0.186%
44	13.404	1920	1923	1927	rVB	20208	23834	1.72%	0.163%
45	13.574	1945	1952	1958	rBV8	18292	48639	3.51%	0.333%
46	13.680	1965	1970	1975	rVB2	23483	37328	2.69%	0.256%
47	13.792	1984	1989	1992	rBV3	32256	58871	4.25%	0.403%
48	13.892	2002	2006	2013	rVB3	42414	71834	5.18%	0.492%
49	14.045	2025	2032	2042	rBV2	489448	874459	63.09%	5.993%
50	14.427	2089	2097	2101	rBV	40955	82295	5.94%	0.564%
51	14.463	2101	2103	2107	rVV	24344	30696	2.21%	0.210%
52	14.521	2110	2113	2116	rVV3	29442	44351	3.20%	0.304%
53	14.557	2116	2119	2126	rVB4	22286	50106	3.62%	0.343%
54	15.086	2204	2209	2218	rBV	91103	212346	15.32%	1.455%
55	15.392	2257	2261	2266	rVB	50056	75822	5.47%	0.520%
56	15.451	2267	2271	2276	rVV	69158	107521	7.76%	0.737%
57	15.515	2277	2282	2295	rVB	241696	421353	30.40%	2.888%
58	16.986	2527	2532	2540	rVB2	27240	62740	4.53%	0.430%
59	17.433	2602	2608	2619	rVB	24602	56511	4.08%	0.387%

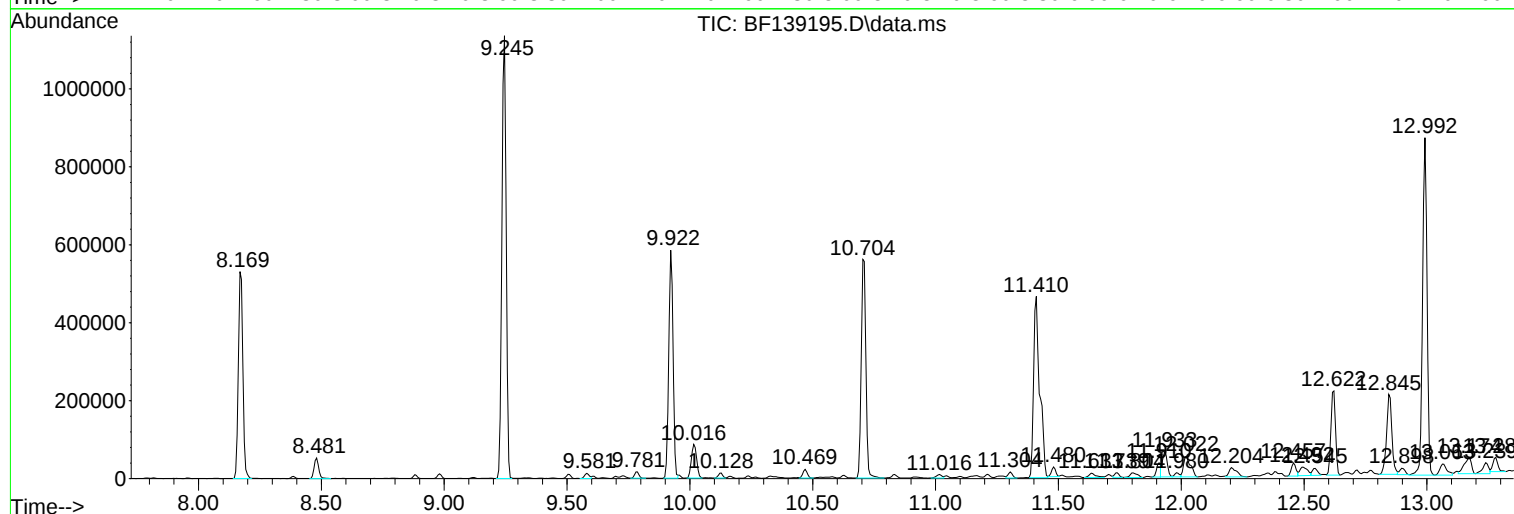
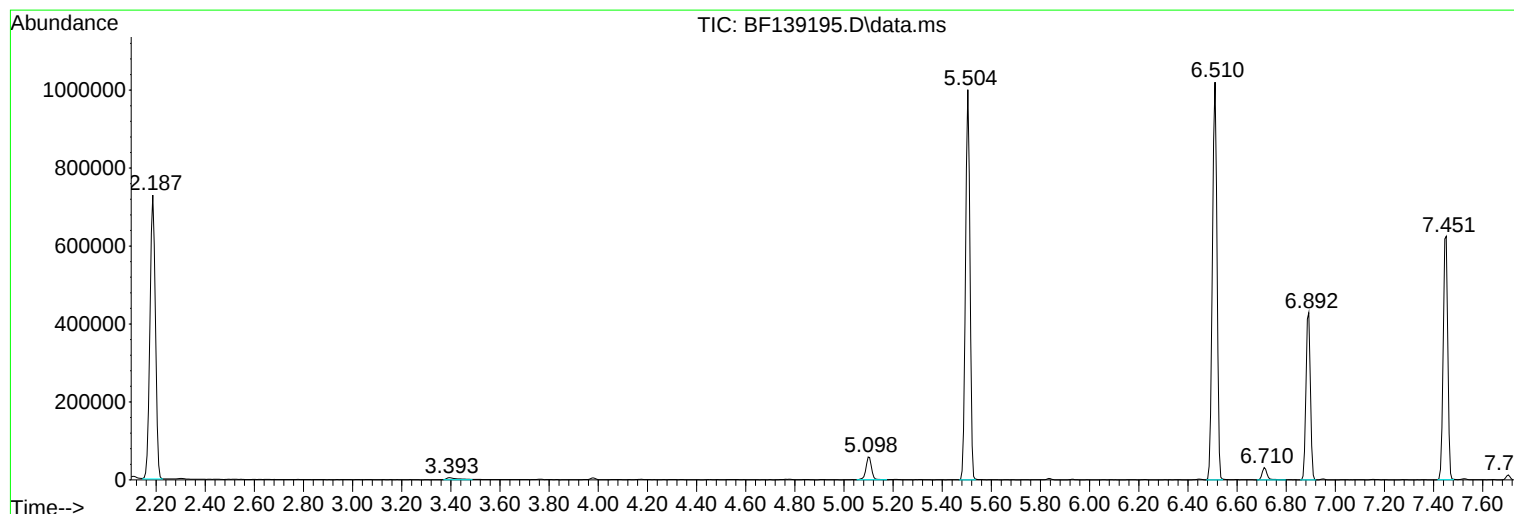
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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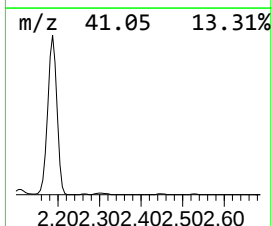
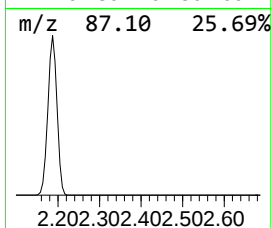
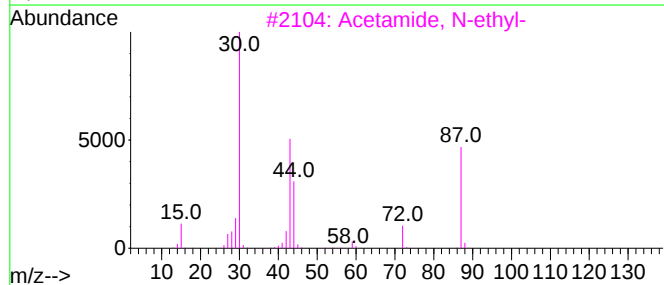
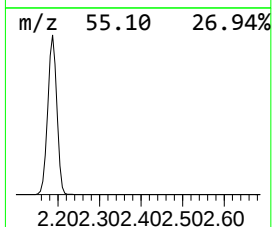
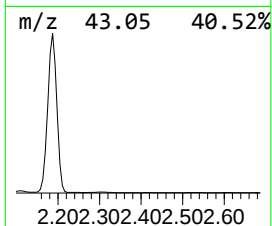
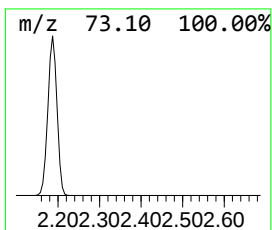
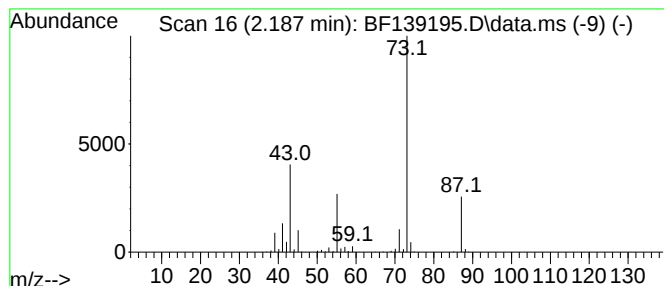
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.187	41.39 ng	1108810	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			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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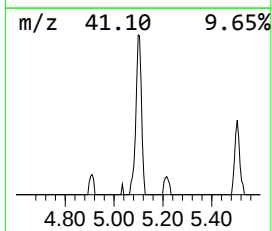
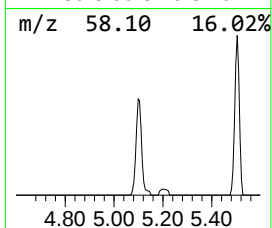
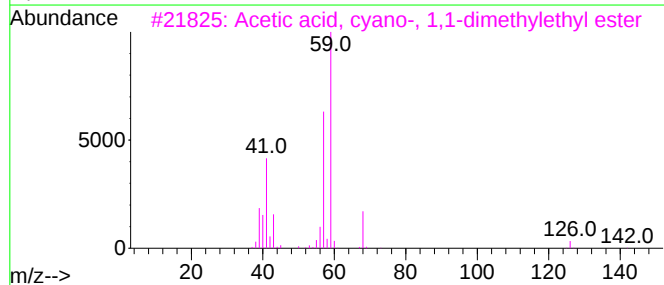
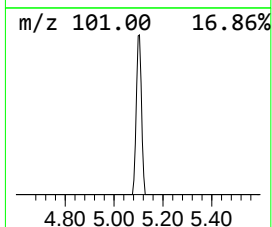
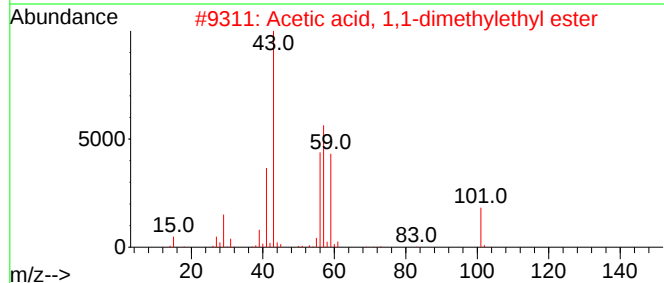
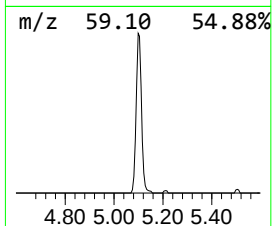
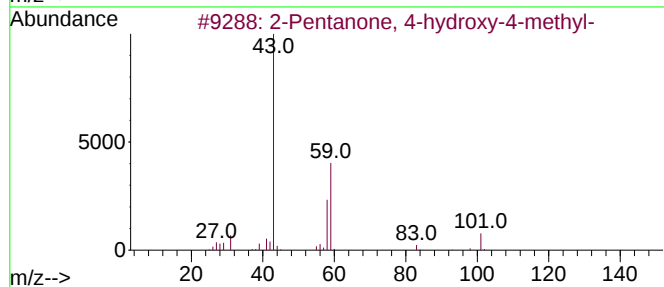
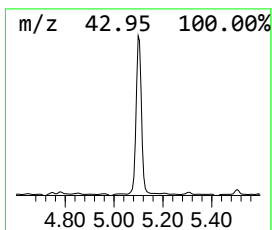
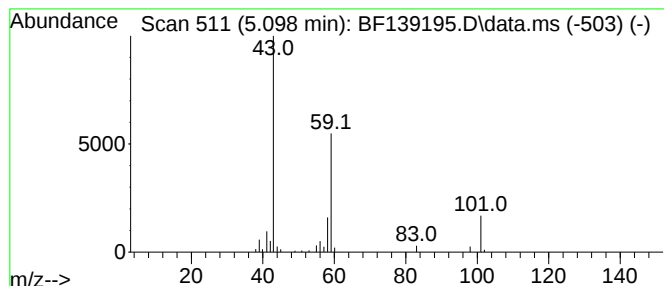
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	3.44 ng	92162	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	50
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	25
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			Acetone	58	C3H6O	000067-64-1	12



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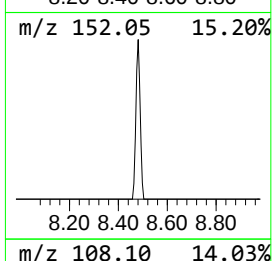
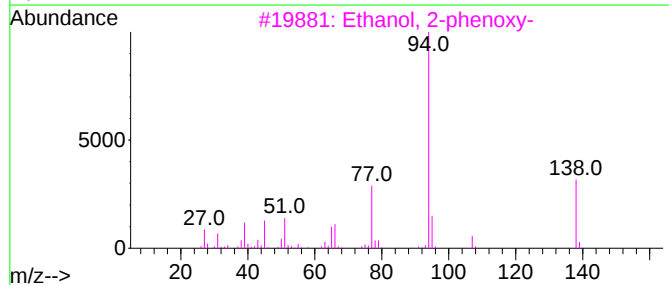
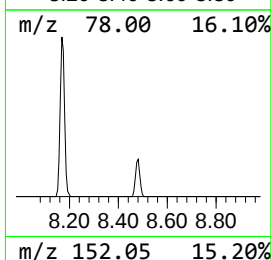
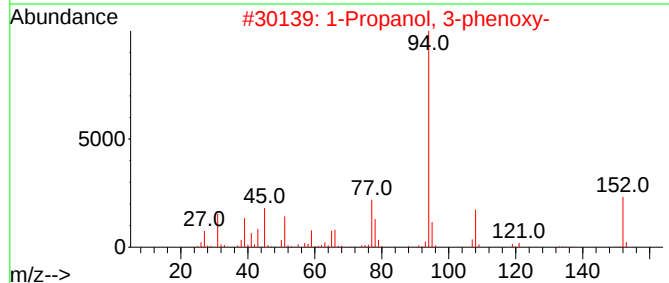
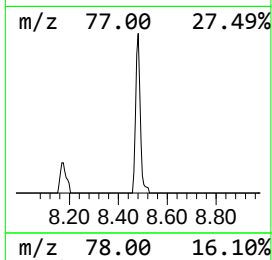
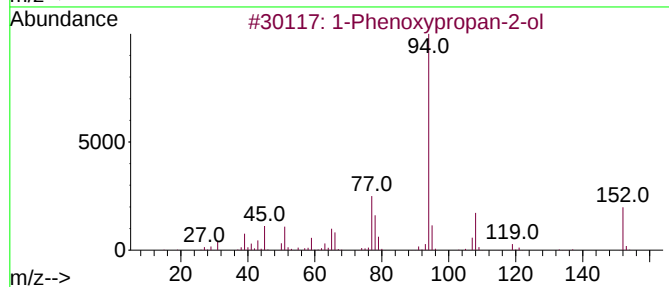
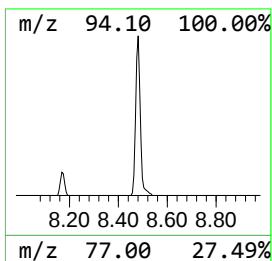
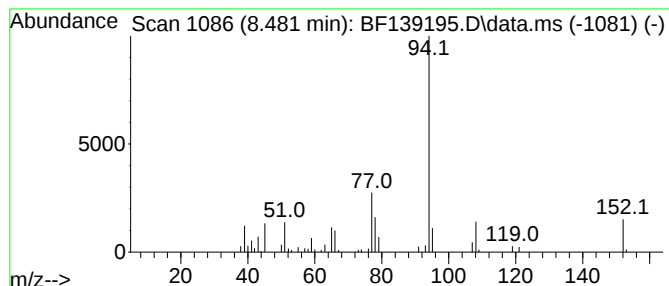
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.481	2.02 ng	68259	Naphthalene-d8	8.169

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	87
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			3-(.alpha.-Hydroxyethyl)-aniline	137	C8H11NO	002454-37-7	59
5			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59



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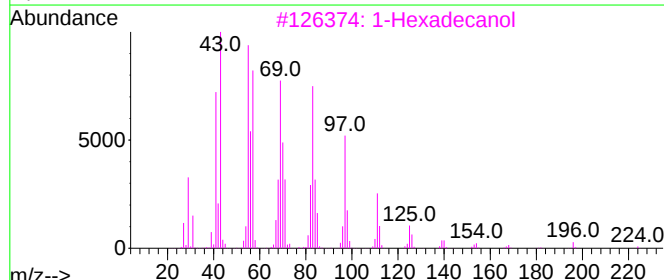
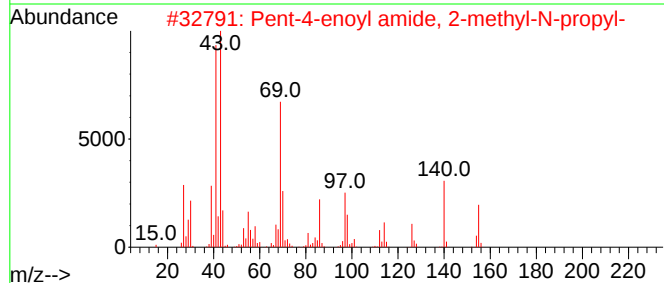
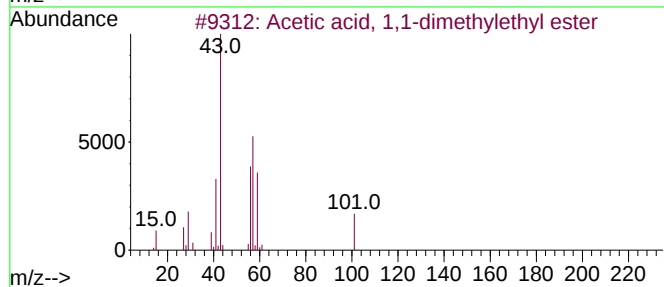
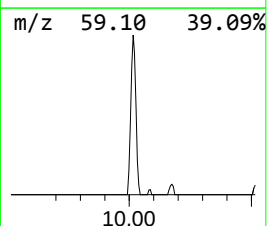
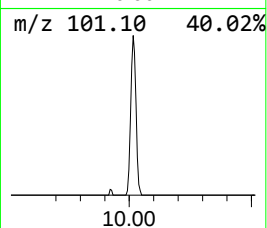
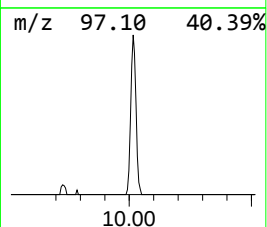
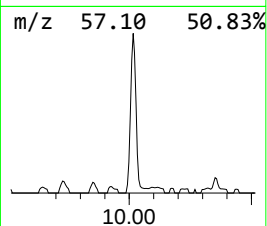
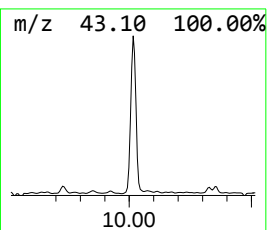
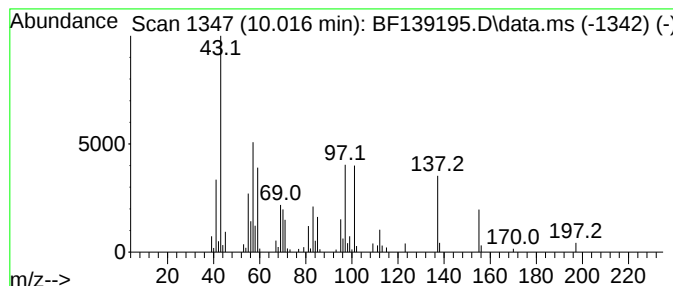
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown10.016 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.016	3.59 ng	128206	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	22
2			Pent-4-enoyl amide, 2-methyl-N-p...	155	C9H17NO	1000420-35-2	14
3			1-Hexadecanol	242	C16H34O	036653-82-4	14
4			7-Oxabicyclo[4.1.0]heptane, 1-me...	112	C7H12O	001713-33-3	10
5			Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	10



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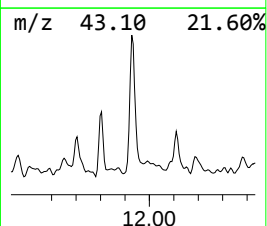
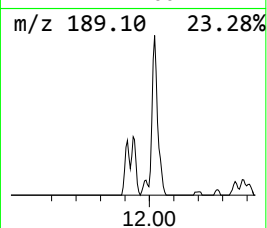
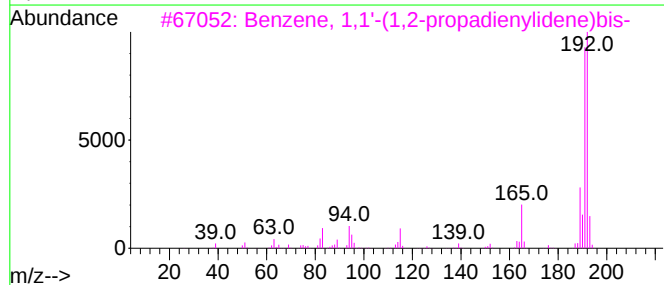
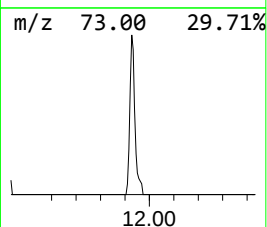
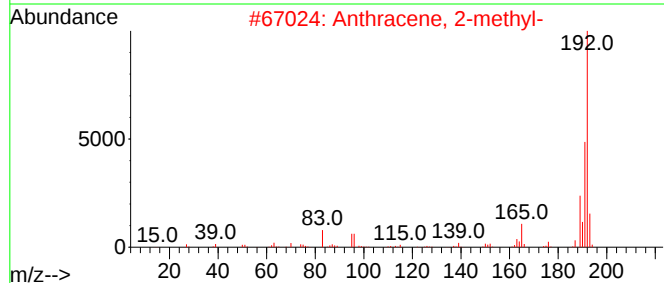
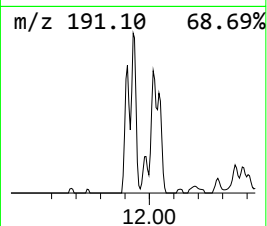
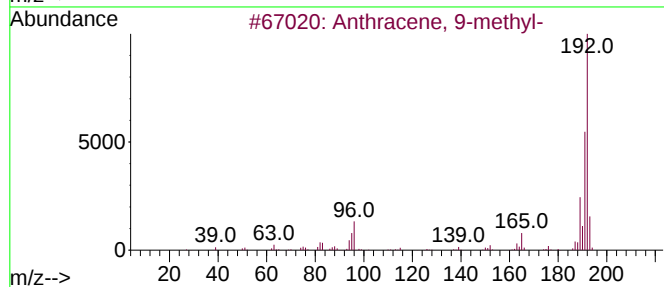
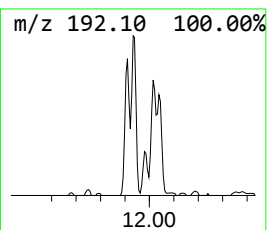
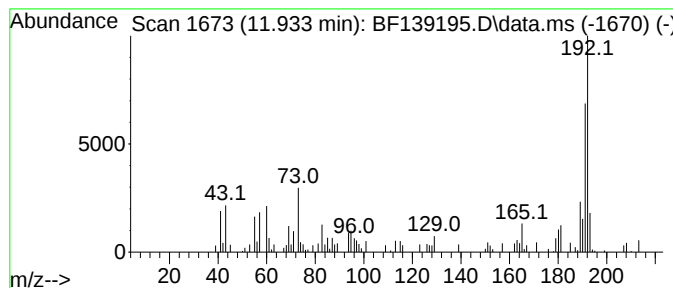
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Anthracene, 9-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	2.18 ng	88224	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 9-methyl-	192	C15H12	000779-02-2	90
2			Anthracene, 2-methyl-	192	C15H12	000613-12-7	78
3			Benzene, 1,1'-(1,2-propadienylid...	192	C15H12	014251-57-1	60
4			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	60
5			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139195.D
Acq On : 27 Aug 2024 19:26
Operator : RC/JU
Sample : P3735-13
Misc :
ALS Vial : 22 Sample Multiplier: 1

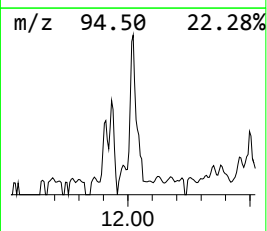
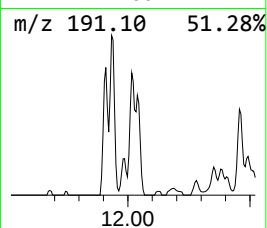
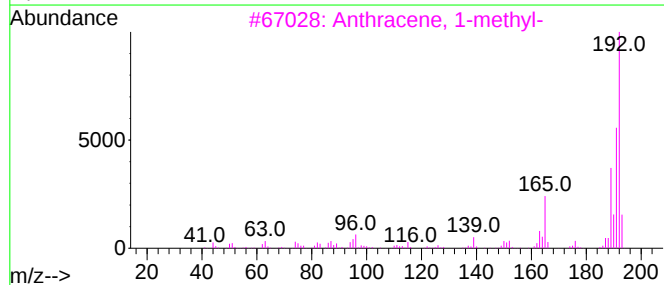
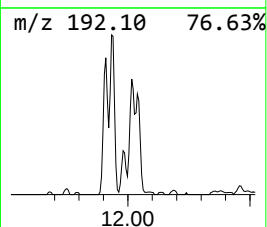
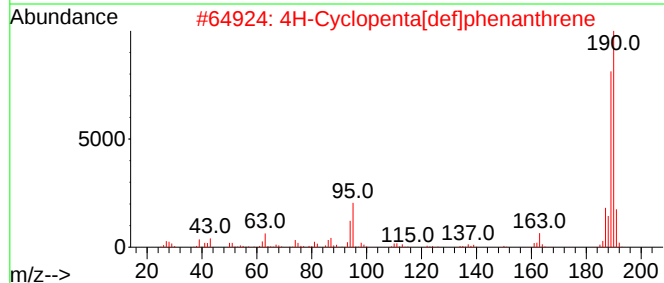
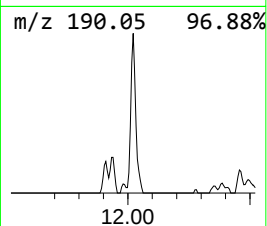
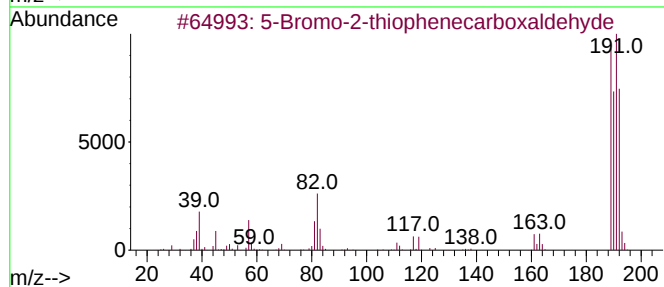
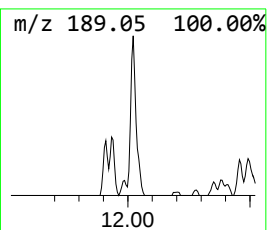
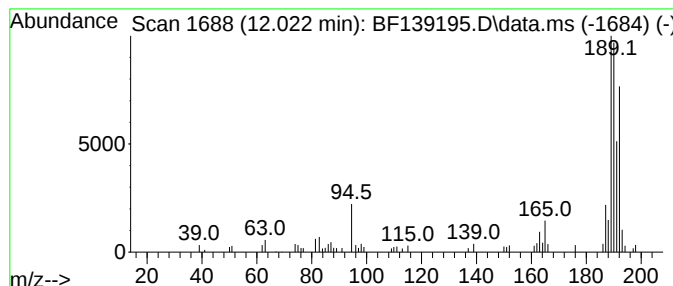
Instrument :
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ClientSampleId :
WC-16

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 5-Bromo-2-thiophenecarboxal... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD			R.T.
12.022	2.56 ng	103883	Phenanthrene-d10			11.410
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	5-Bromo-2-thiophenecarboxaldehyde		190	C5H3BrOS	004701-17-1	58
2	4H-Cyclopenta[def]phenanthrene		190	C15H10	000203-64-5	55
3	Anthracene, 1-methyl-		192	C15H12	000610-48-0	42
4	5H-Dibenzo[a,d]cycloheptene		192	C15H12	000256-81-5	42
5	Phenanthrene, 1-methyl-		192	C15H12	000832-69-9	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139195.D
Acq On : 27 Aug 2024 19:26
Operator : RC/JU
Sample : P3735-13
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-16

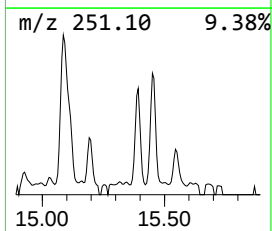
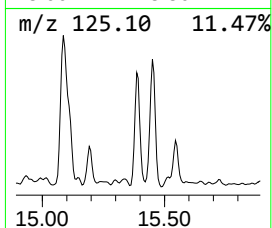
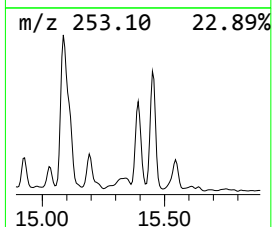
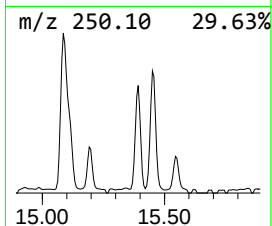
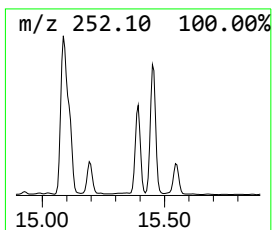
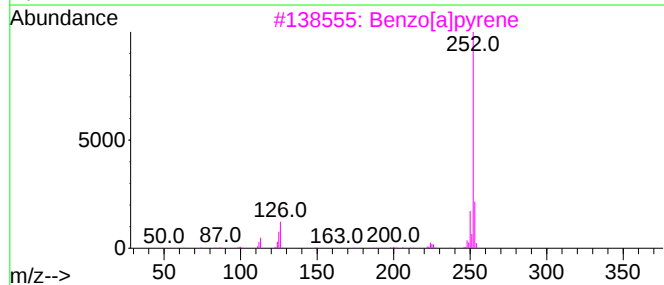
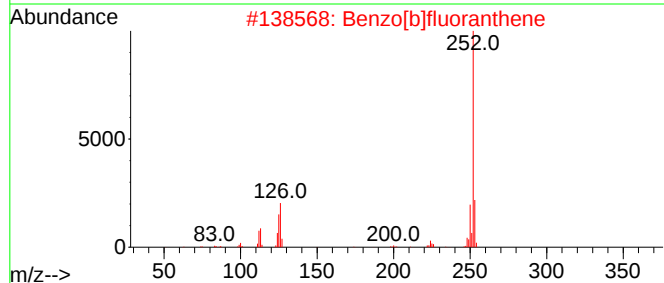
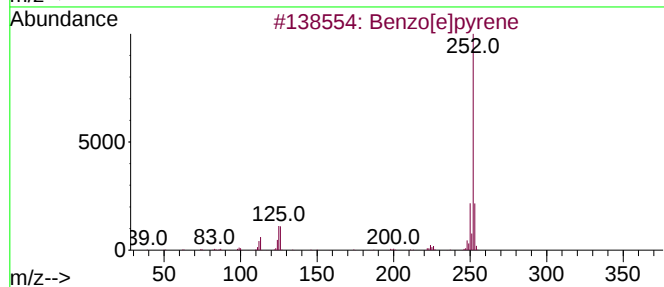
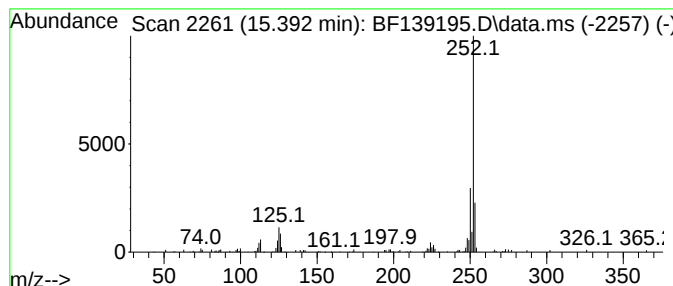
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.392	3.60 ng	75822	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	94
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
3			Benzo[a]pyrene	252	C20H12	000050-32-8	91
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	91
5			Perylene	252	C20H12	000198-55-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139195.D
Acq On : 27 Aug 2024 19:26
Operator : RC/JU
Sample : P3735-13
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-16

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.187	41.4	ng	1108810	1	6.892	535847	20.0
2-Pentanone, 4-...	5.098	3.4	ng	92162	1	6.892	535847	20.0
1-Phenoxypropan...	8.481	2.0	ng	68259	2	8.169	677151	20.0
unknown10.016	10.016	3.6	ng	128206	3	9.922	714493	20.0
Anthracene, 9-m...	11.933	2.2	ng	88224	4	11.410	810603	20.0
5-Bromo-2-thiop...	12.022	2.6	ng	103883	4	11.410	810603	20.0
Benzo[e]pyrene	15.392	3.6	ng	75822	6	15.515	421353	20.0