

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120324\
 Data File : BF140717.D
 Acq On : 03 Dec 2024 18:00
 Operator : RC/JU
 Sample : P5052-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OR-640-COMP-50

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-BF112124.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140717.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	20	rVB	626558	980893	56.35%	5.594%
2	2.257	23	28	39	rVB	24663	41251	2.37%	0.235%
3	5.092	505	510	528	rVB	73830	115930	6.66%	0.661%
4	5.504	574	580	605	rBV	954962	1301390	74.76%	7.421%
5	6.510	745	751	773	rBV	1009538	1371839	78.80%	7.823%
6	6.869	807	812	820	rBV	367490	446099	25.63%	2.544%
7	7.433	902	908	918	rBV	656750	885631	50.87%	5.050%
8	7.686	946	951	962	rBV	19391	37622	2.16%	0.215%
9	8.151	1024	1030	1047	rBV	428747	575653	33.07%	3.283%
10	9.222	1207	1212	1222	rBV	1399169	1740828	100.00%	9.927%
11	9.904	1323	1328	1332	rBV	509491	637674	36.63%	3.636%
12	10.616	1444	1449	1458	rBV	181567	228317	13.12%	1.302%
13	10.698	1458	1463	1477	rBV	726555	960100	55.15%	5.475%
14	11.204	1545	1549	1553	rBV	16526	20927	1.20%	0.119%
15	11.292	1559	1564	1568	rVB	15400	19384	1.11%	0.111%
16	11.398	1576	1582	1584	rBV	474629	710877	40.84%	4.054%
17	11.416	1584	1585	1590	rVV	398353	408503	23.47%	2.329%
18	11.469	1590	1594	1600	rVB2	47387	74138	4.26%	0.423%
19	11.633	1615	1622	1627	rBV2	48023	75509	4.34%	0.431%
20	11.921	1663	1671	1678	rBV3	79922	168791	9.70%	0.963%
21	12.010	1682	1686	1694	rVB2	48315	85884	4.93%	0.490%
22	12.192	1714	1717	1720	rBV	17782	20384	1.17%	0.116%
23	12.227	1720	1723	1727	rVB	37048	43285	2.49%	0.247%
24	12.486	1763	1767	1772	rVB4	10831	17954	1.03%	0.102%
25	12.539	1772	1776	1783	rVB	26894	35003	2.01%	0.200%
26	12.616	1783	1789	1794	rBV	700499	888759	51.05%	5.068%
27	12.763	1808	1814	1820	rBV2	22719	40492	2.33%	0.231%
28	12.845	1820	1828	1833	rVV	539619	802887	46.12%	4.578%
29	12.892	1833	1836	1840	rVB	18137	24409	1.40%	0.139%
30	12.980	1844	1851	1860	rBV	1045350	1382201	79.40%	7.882%
31	13.057	1860	1864	1869	rBV4	21538	38282	2.20%	0.218%
32	13.168	1875	1883	1887	rBV2	30684	78230	4.49%	0.446%
33	13.274	1897	1901	1909	rBV3	25129	56941	3.27%	0.325%
34	13.404	1920	1923	1930	rVB4	12995	23481	1.35%	0.134%
35	13.545	1943	1947	1954	rBV3	13953	25705	1.48%	0.147%
36	13.692	1967	1972	1978	rVB	41538	57148	3.28%	0.326%

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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-BF112124.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.798	1986	1990	1993	rBV	43966	66433	3.82%	0.379%
38	13.874	1997	2003	2006	rBV4	66519	124728	7.16%	0.711%
39	14.051	2025	2033	2037	rBV2	442635	837057	48.08%	4.773%
40	14.162	2049	2052	2056	rBV	27184	35888	2.06%	0.205%
41	14.974	2186	2190	2198	rBV3	19398	37955	2.18%	0.216%
42	15.139	2212	2218	2229	rBV	270327	613713	35.25%	3.500%
43	15.251	2233	2237	2242	rVV	25219	34778	2.00%	0.198%
44	15.445	2266	2270	2277	rVB	131792	218977	12.58%	1.249%
45	15.515	2277	2282	2287	rVB	174142	266815	15.33%	1.522%
46	15.574	2287	2292	2297	rBV	284813	466000	26.77%	2.657%
47	17.092	2543	2550	2561	rBV2	101930	238382	13.69%	1.359%
48	17.550	2622	2628	2639	rVB	73928	172981	9.94%	0.986%

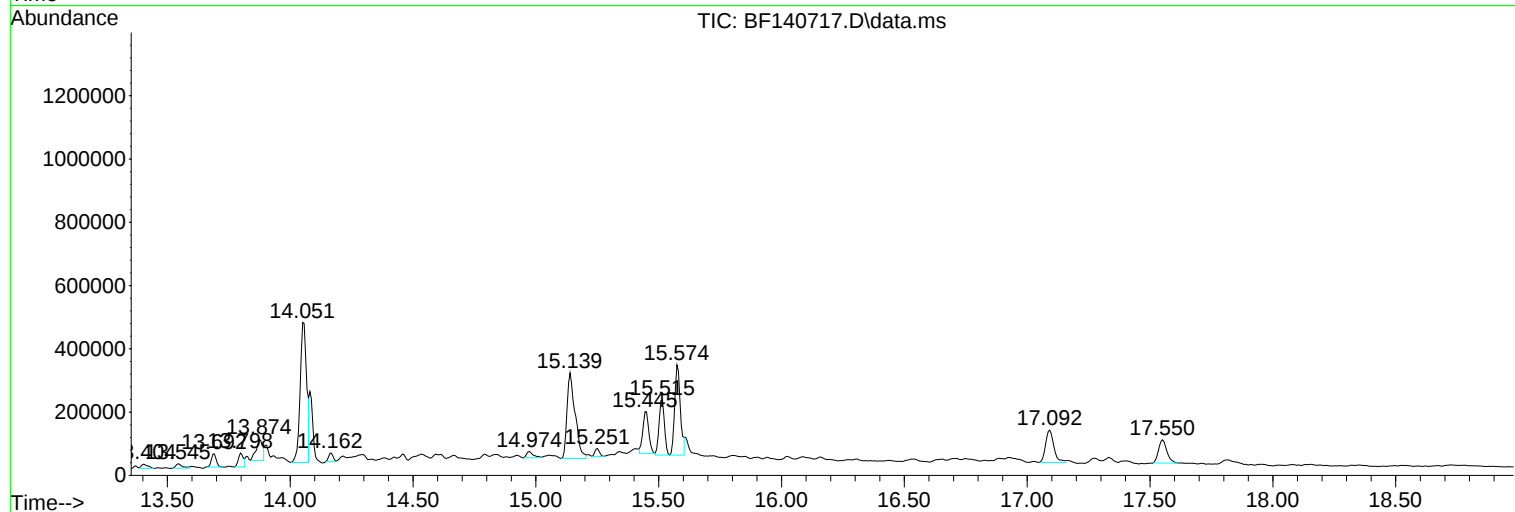
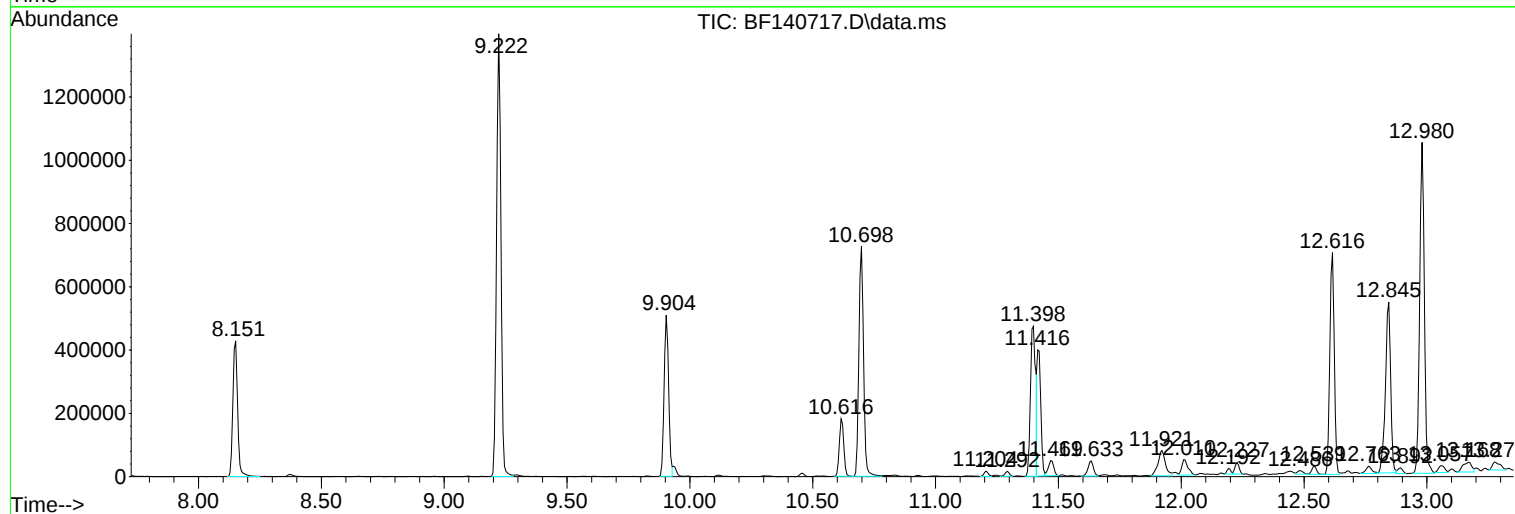
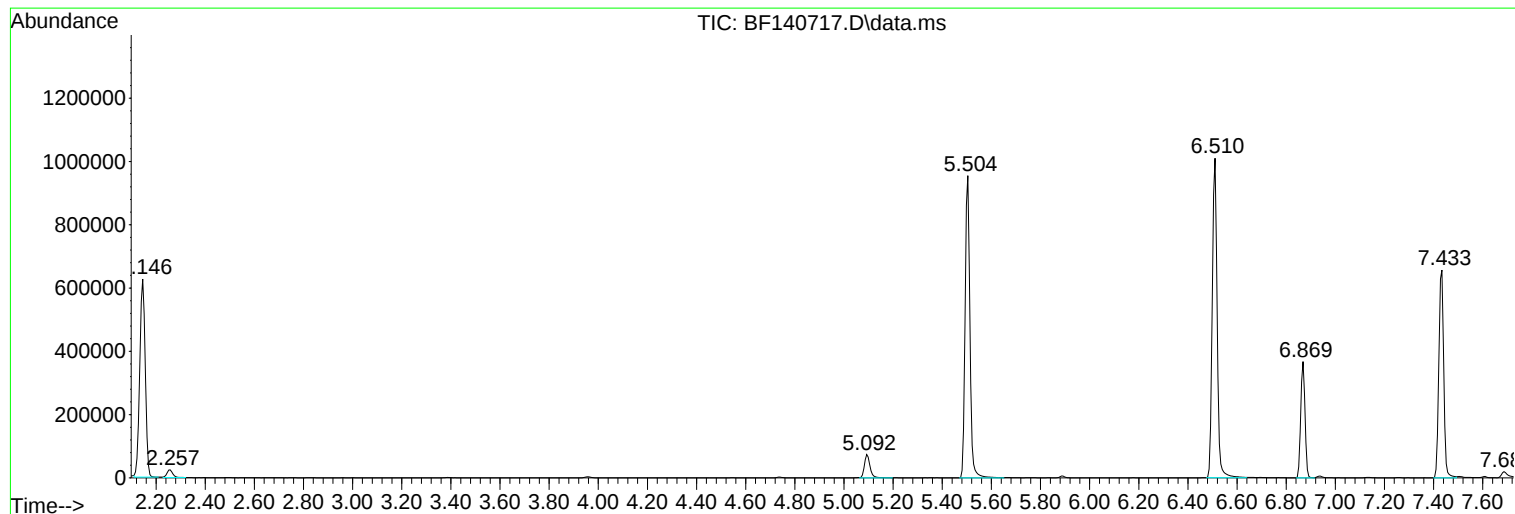
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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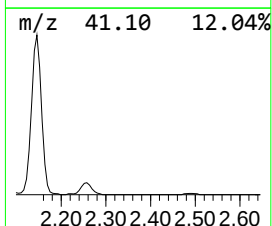
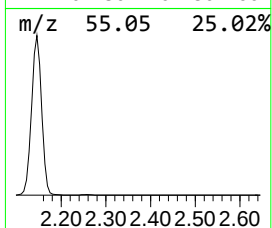
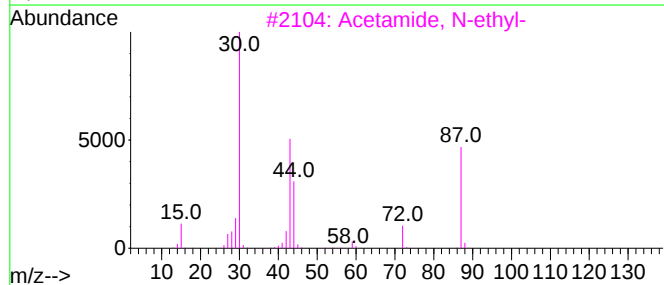
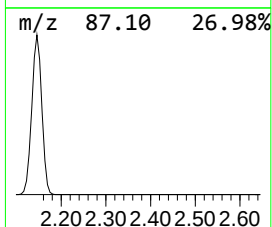
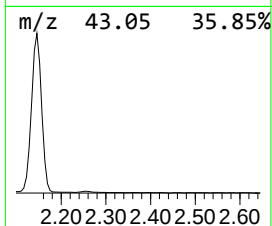
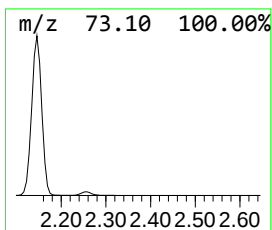
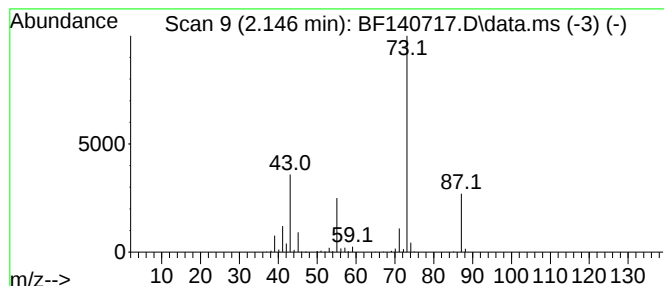
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	43.98 ng	980893	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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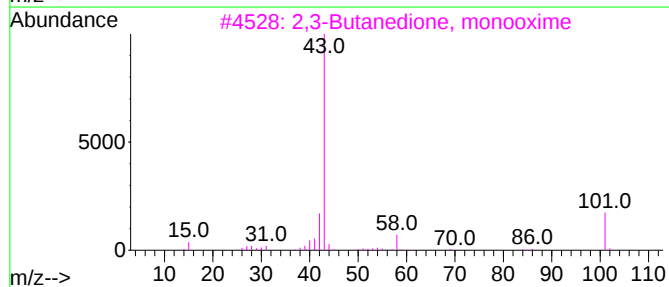
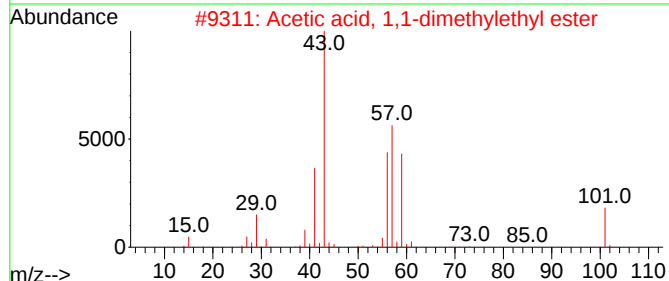
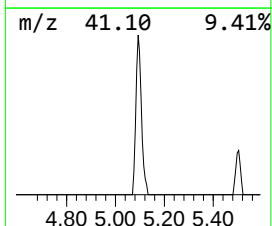
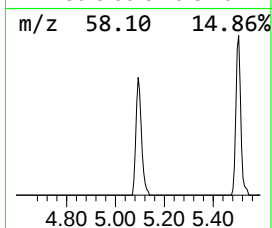
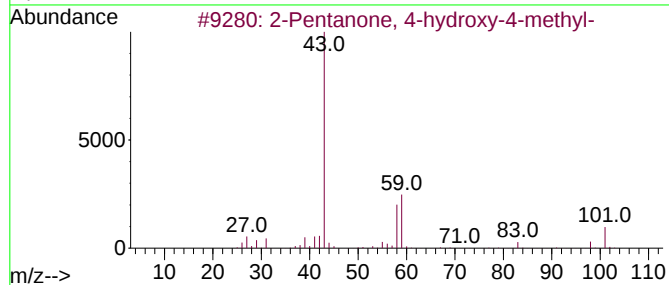
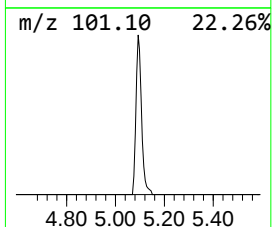
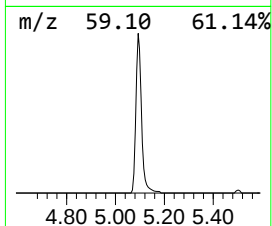
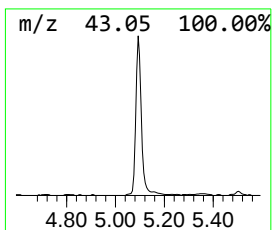
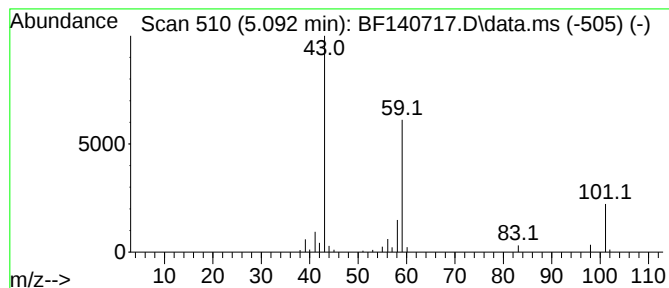
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.092	5.20 ng	115930	1,4-Dichlorobenzene-d4	6.869

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	39
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4			3-Hexanol	102	C6H14O	000623-37-0	28
5			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25



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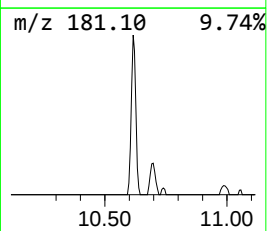
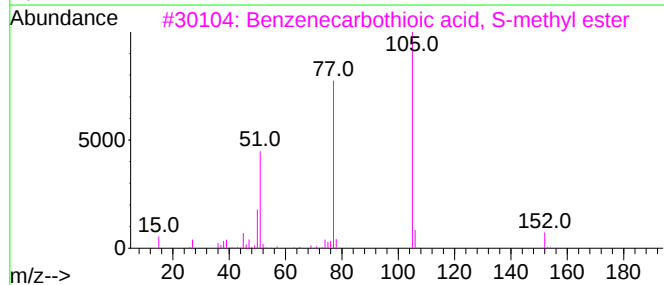
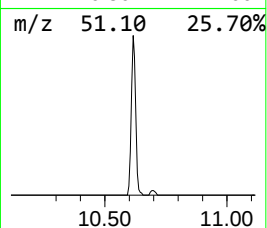
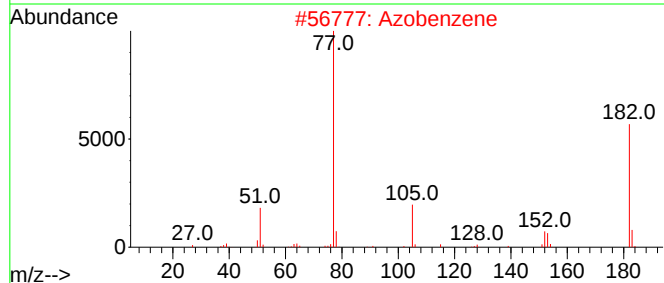
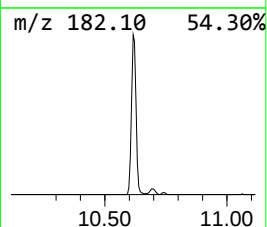
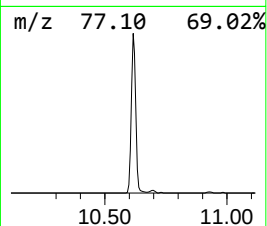
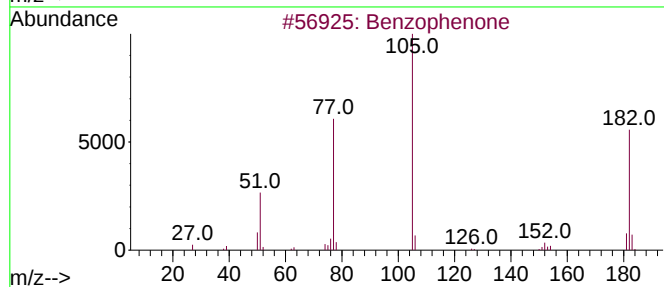
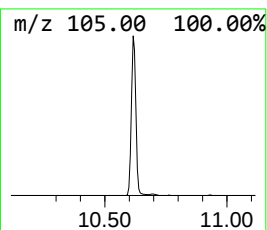
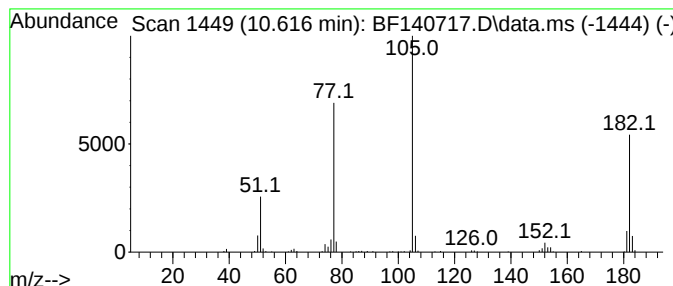
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.616	7.16 ng	228317	Acenaphthene-d10	9.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	64
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
4			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
5			Benzoyl bromide	184	C7H5BrO	000618-32-6	47



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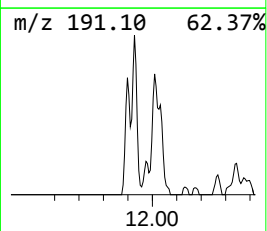
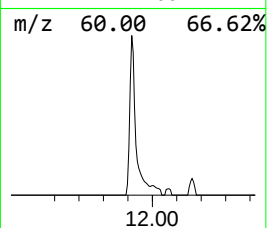
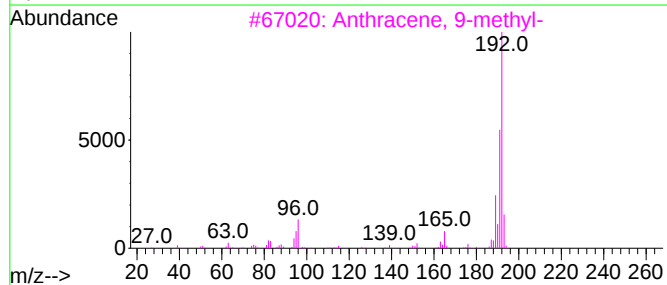
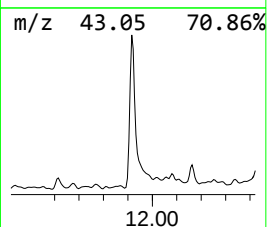
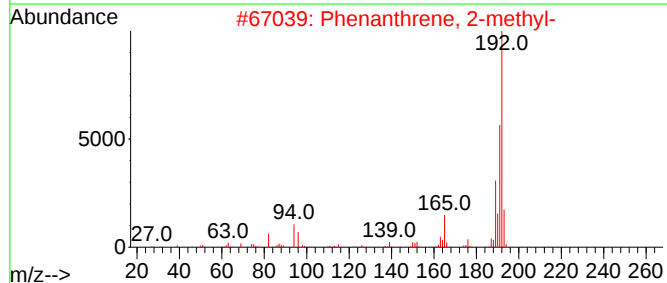
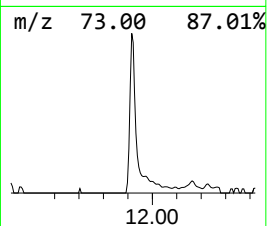
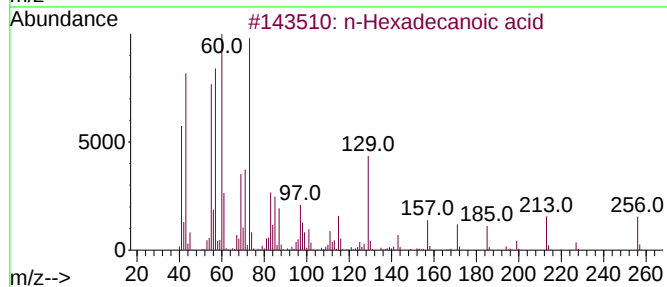
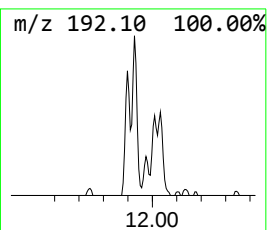
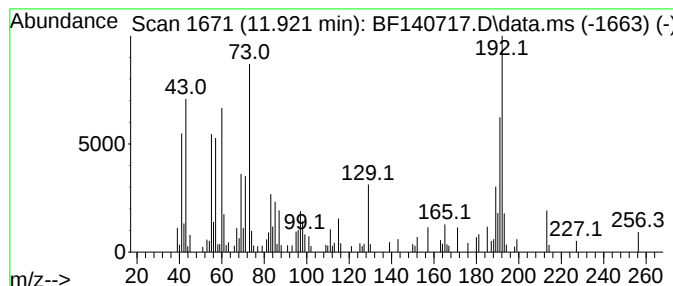
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.921	4.75 ng	168791	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	86
3			Anthracene, 9-methyl-	192	C15H12	000779-02-2	81
4			Anthracene, 1-methyl-	192	C15H12	000610-48-0	80
5			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	49



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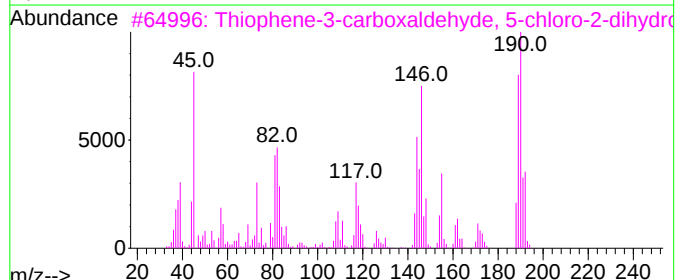
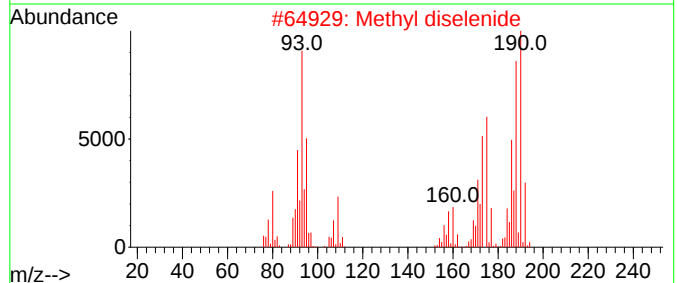
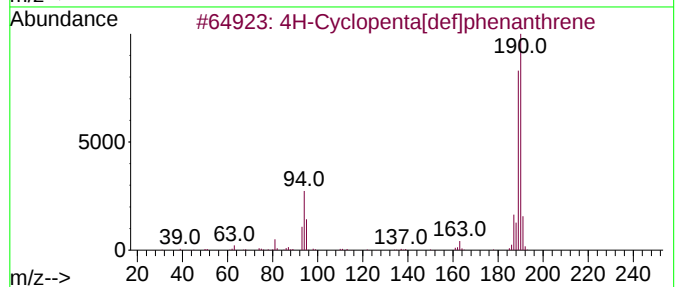
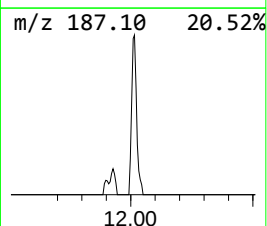
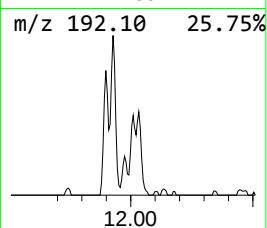
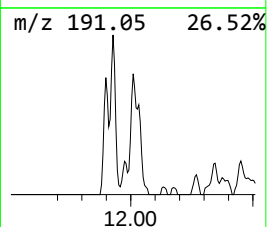
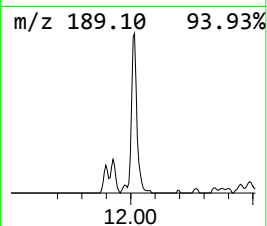
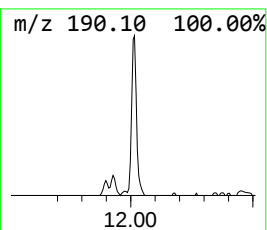
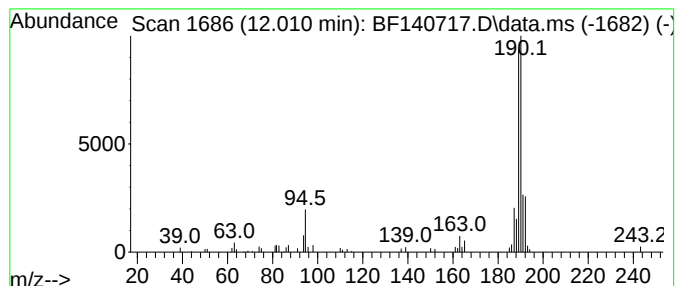
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.010	2.42 ng	85884	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2			Methyl diselenide	190	C2H6Se2	007101-31-7	53
3			Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	52
4			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
5			2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120324\
Data File : BF140717.D
Acq On : 03 Dec 2024 18:00
Operator : RC/JU
Sample : P5052-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-640-COMP-50

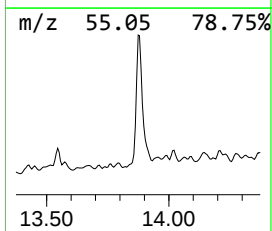
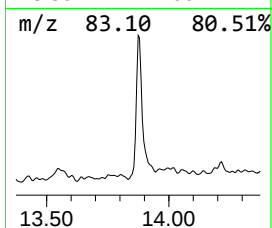
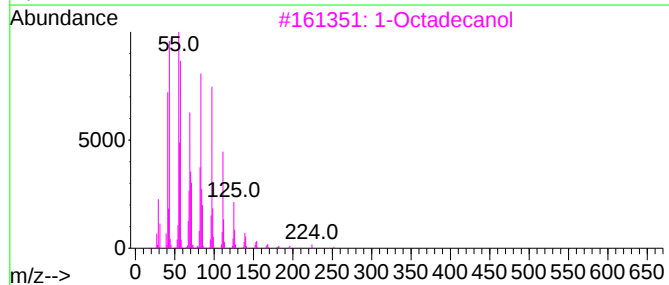
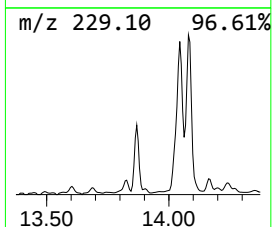
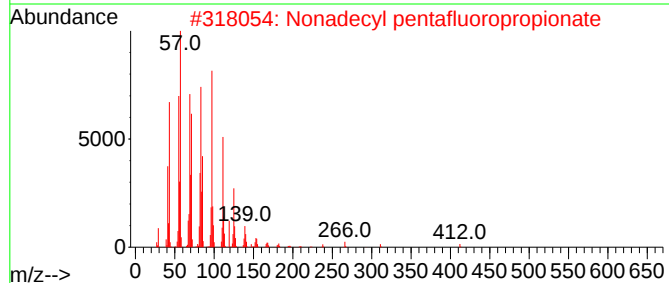
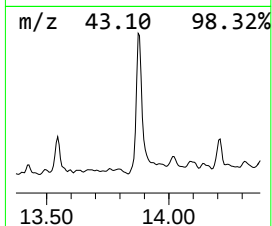
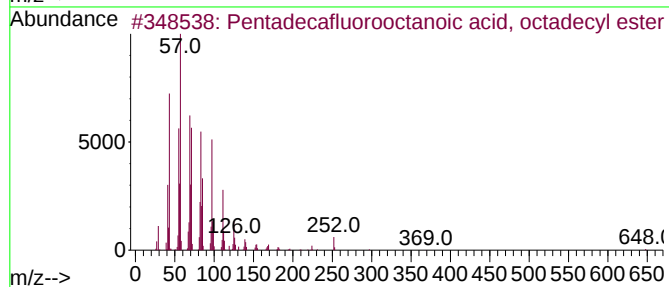
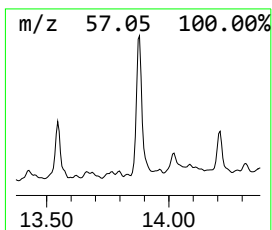
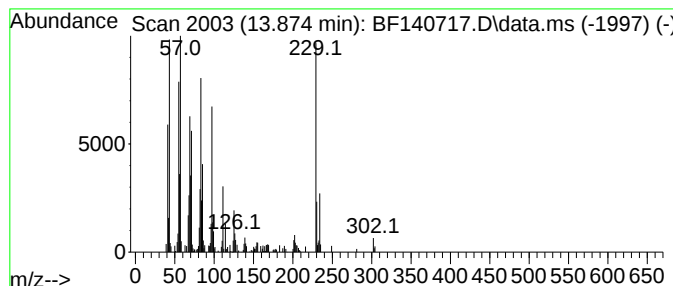
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentadecafluorooctanoic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	2.98 ng	124728	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	78
2			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	60
3			1-Octadecanol	270	C18H38O	000112-92-5	55
4			1-Heneicosanol	312	C21H44O	015594-90-8	55
5			1-Tricosene	322	C23H46	018835-32-0	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120324\
Data File : BF140717.D
Acq On : 03 Dec 2024 18:00
Operator : RC/JU
Sample : P5052-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-640-COMP-50

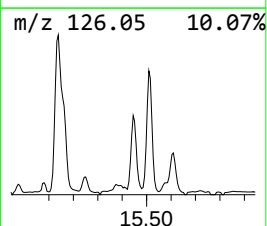
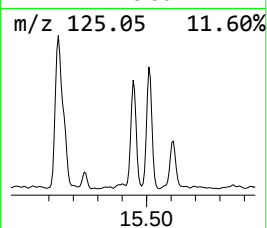
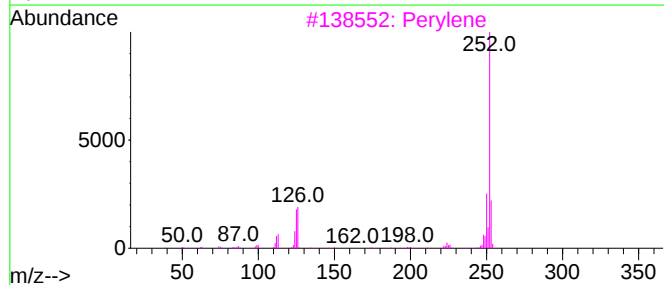
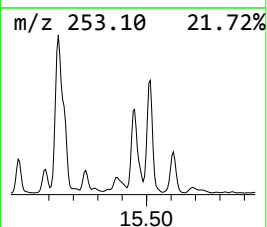
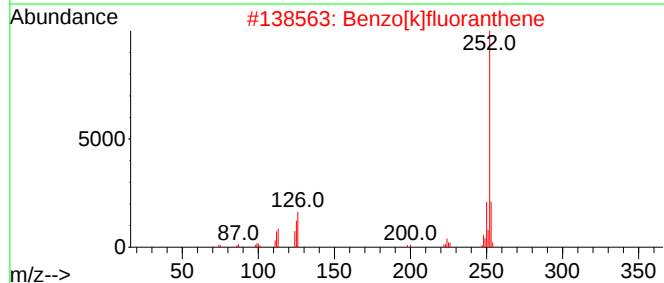
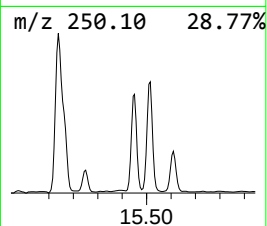
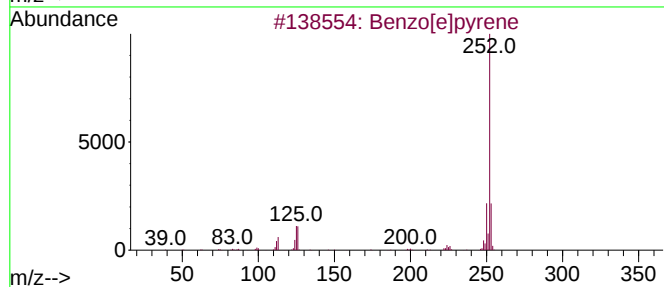
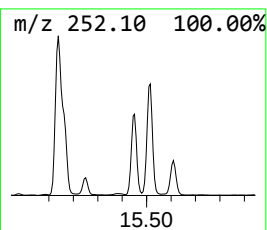
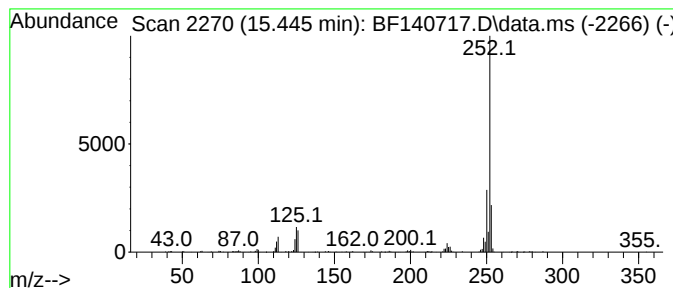
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.445	9.40 ng	218977	Perylene-d12	15.574

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	95
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120324\
Data File : BF140717.D
Acq On : 03 Dec 2024 18:00
Operator : RC/JU
Sample : P5052-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-640-COMP-50

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.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	44.0	ng	980893	1	6.869	446099	20.0
2-Pentanone, 4-...	5.092	5.2	ng	115930	1	6.869	446099	20.0
Benzophenone	10.616	7.2	ng	228317	3	9.904	637674	20.0
n-Hexadecanoic ...	11.921	4.8	ng	168791	4	11.398	710877	20.0
4H-Cyclopenta[d...]	12.010	2.4	ng	85884	4	11.398	710877	20.0
Pentadecafluoro...	13.874	3.0	ng	124728	5	14.057	837057	20.0
Benzo[e]pyrene	15.445	9.4	ng	218977	6	15.574	466000	20.0