

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102924\
 Data File : BF140125.D
 Acq On : 29 Oct 2024 21:13
 Operator : RC/JU
 Sample : P4578-04
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WB-305-TOP-1

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-BF101824.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140125.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	9	17	25	rVB	1088074	1758043	71.25%	7.928%
2	3.999	318	324	332	rBV	26173	41287	1.67%	0.186%
3	5.122	505	515	520	rVB2	17224	31171	1.26%	0.141%
4	5.510	574	581	586	rBV	1648997	2257782	91.50%	10.182%
5	6.510	744	751	760	rBV	1646359	2345106	95.04%	10.576%
6	6.887	810	815	821	rBV	609379	754398	30.57%	3.402%
7	7.281	876	882	888	rBV2	19713	31166	1.26%	0.141%
8	7.445	901	910	915	rBV	1149031	1535698	62.24%	6.926%
9	7.651	939	945	947	rBV2	19479	29157	1.18%	0.131%
10	7.698	947	953	958	rVB2	68012	117577	4.77%	0.530%
11	7.904	981	988	993	rBV3	32616	57208	2.32%	0.258%
12	8.169	1025	1033	1040	rBV	790526	1086753	44.04%	4.901%
13	8.381	1064	1069	1074	rVB	22820	29587	1.20%	0.133%
14	8.757	1129	1133	1137	rVB	28555	32499	1.32%	0.147%
15	8.881	1150	1154	1158	rVB	52076	61979	2.51%	0.280%
16	8.981	1166	1171	1176	rVB	55762	68391	2.77%	0.308%
17	9.245	1210	1216	1221	rBV	1861894	2467471	100.00%	11.128%
18	9.322	1225	1229	1238	rVB	34980	54911	2.23%	0.248%
19	9.439	1245	1249	1255	rVB	25365	38396	1.56%	0.173%
20	9.504	1255	1260	1265	rBV	27995	43152	1.75%	0.195%
21	9.581	1268	1273	1276	rVV	48747	72916	2.96%	0.329%
22	9.639	1280	1283	1290	rVB3	23533	33547	1.36%	0.151%
23	9.698	1290	1293	1302	rVB	26992	41218	1.67%	0.186%
24	9.781	1303	1307	1311	rVB	29818	38729	1.57%	0.175%
25	9.851	1312	1319	1323	rVB2	20368	30786	1.25%	0.139%
26	9.922	1323	1331	1335	rBV	817926	1056036	42.80%	4.762%
27	9.957	1335	1337	1341	rVB	54373	53837	2.18%	0.243%
28	10.122	1361	1365	1369	rBV3	23629	32062	1.30%	0.145%
29	10.239	1380	1385	1388	rBV2	21928	34086	1.38%	0.154%
30	10.328	1396	1400	1406	rBV4	21879	49834	2.02%	0.225%
31	10.469	1421	1424	1429	rVB2	30697	39082	1.58%	0.176%
32	10.575	1437	1442	1447	rVV3	27728	58376	2.37%	0.263%
33	10.633	1447	1452	1459	rVV	391177	501396	20.32%	2.261%
34	10.710	1459	1465	1477	rVV	881778	1150978	46.65%	5.191%
35	10.833	1481	1486	1493	rVB	42768	71871	2.91%	0.324%
36	10.945	1501	1505	1509	rBV	23217	28240	1.14%	0.127%

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37	11.016	1512	1517	1520	rBV3	26625	41409	1.68%	0.187%
38	11.304	1563	1566	1572	rVB2	34728	49619	2.01%	0.224%
39	11.410	1579	1584	1592	rBV2	665165	984176	39.89%	4.438%
40	11.480	1592	1596	1600	rVB	45007	62774	2.54%	0.283%
41	11.933	1665	1673	1679	rBV2	211475	375151	15.20%	1.692%
42	12.022	1685	1688	1697	rVB	83676	174038	7.05%	0.785%
43	12.463	1759	1763	1766	rBV	33039	39648	1.61%	0.179%
44	12.498	1766	1769	1775	rVB2	29925	47729	1.93%	0.215%
45	12.557	1775	1779	1786	rVB4	19367	42834	1.74%	0.193%
46	12.622	1786	1790	1794	rBV	104452	145188	5.88%	0.655%
47	12.663	1794	1797	1803	rVB	146157	185046	7.50%	0.835%
48	12.716	1803	1806	1814	rVB	43486	60423	2.45%	0.272%
49	12.851	1825	1829	1835	rVB	111655	155023	6.28%	0.699%
50	12.998	1848	1854	1862	rVB	1243943	1626866	65.93%	7.337%
51	13.074	1863	1867	1874	rVV2	20130	37320	1.51%	0.168%
52	13.180	1879	1885	1889	rVB	41687	72574	2.94%	0.327%
53	13.286	1900	1903	1910	rVB2	25780	38825	1.57%	0.175%
54	13.898	2002	2007	2015	rBV	74421	135355	5.49%	0.610%
55	13.969	2016	2019	2025	rVB4	24151	29976	1.21%	0.135%
56	14.051	2027	2033	2045	rBV2	544721	870255	35.27%	3.925%
57	15.110	2209	2213	2221	rVB	37266	81467	3.30%	0.367%
58	15.416	2262	2265	2271	rVB	29110	43379	1.76%	0.196%
59	15.480	2272	2276	2281	rVV	44652	69894	2.83%	0.315%
60	15.545	2281	2287	2300	rVB	411809	670432	27.17%	3.023%

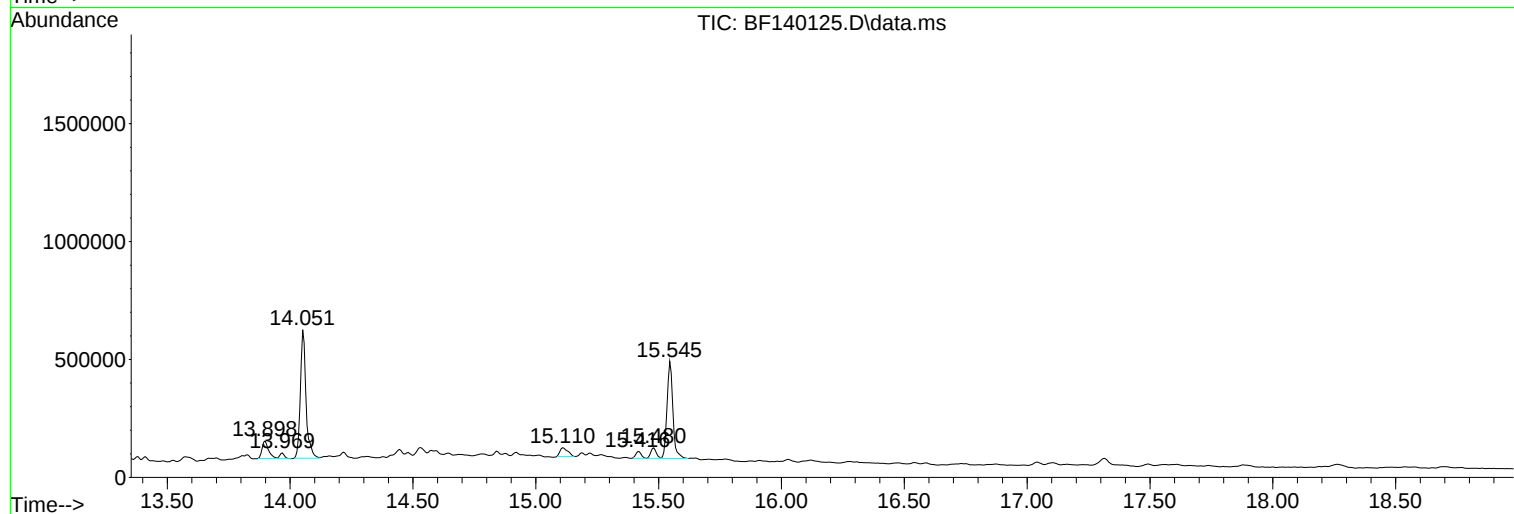
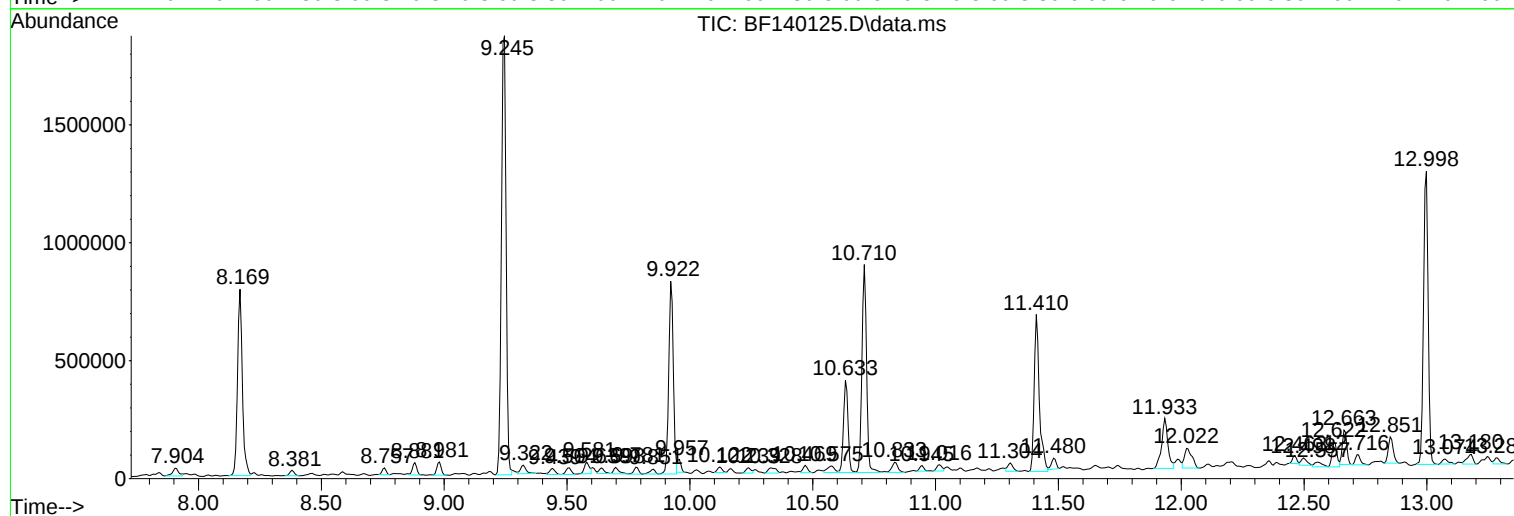
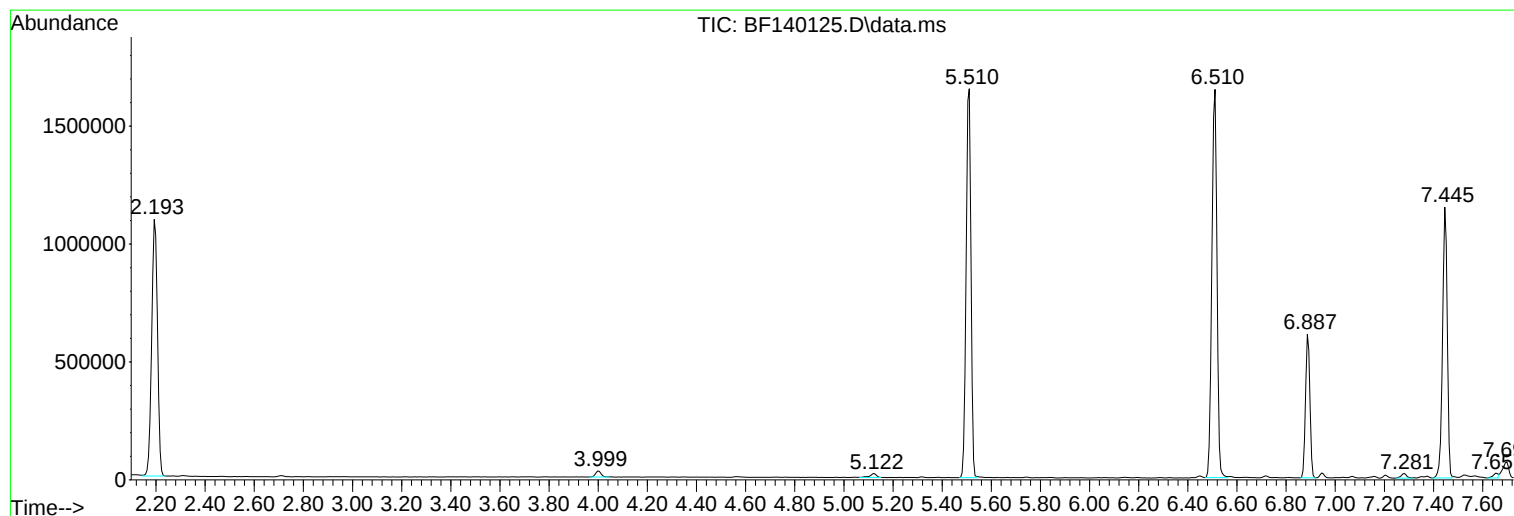
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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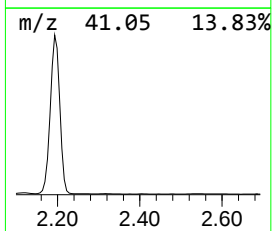
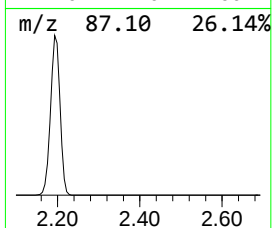
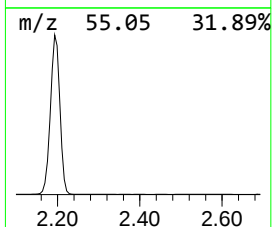
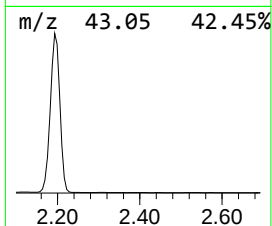
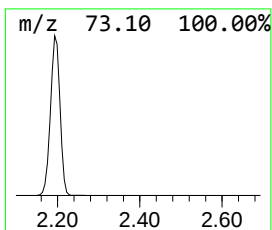
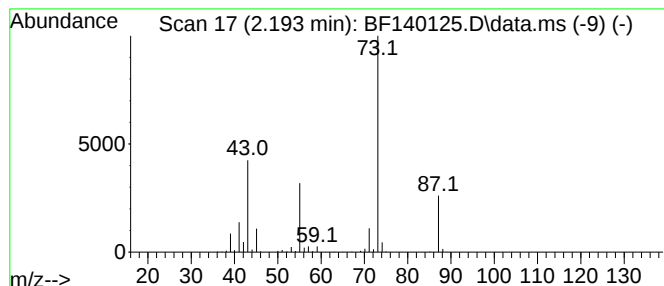
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.193	46.61 ng	1758040	1,4-Dichlorobenzene-d4	6.887

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			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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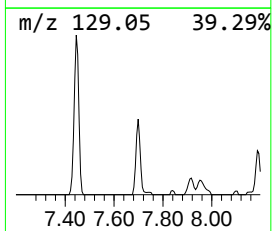
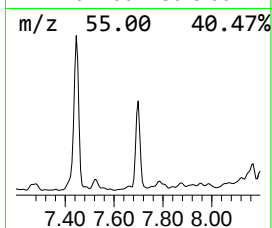
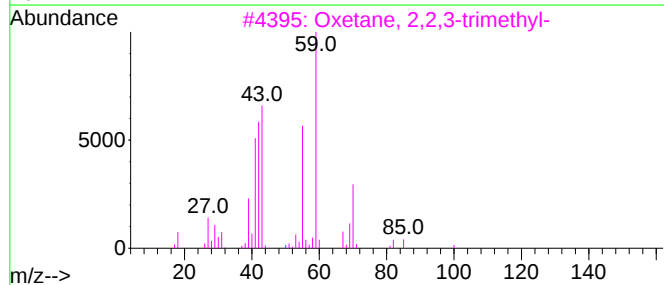
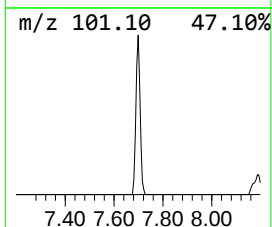
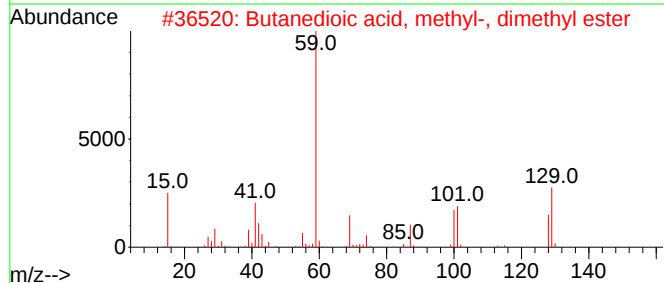
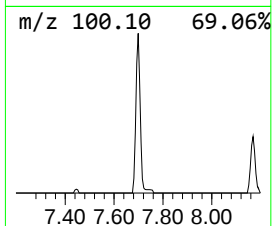
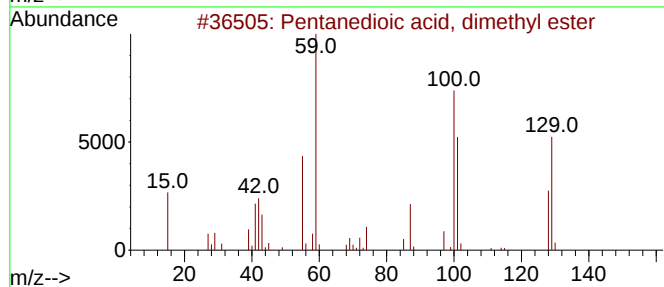
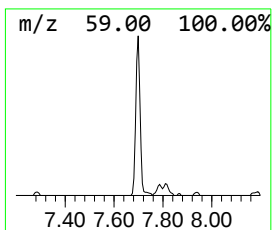
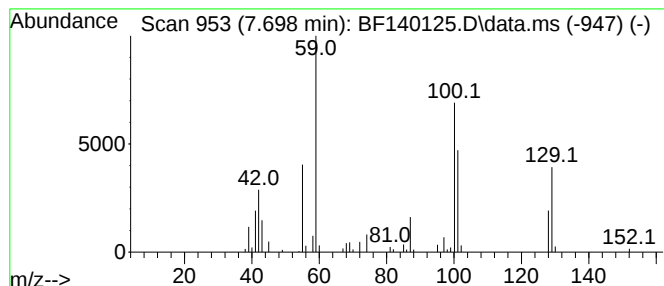
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Pentanedioic acid, dimethyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.698	2.16 ng	117577	Naphthalene-d8	8.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	91
2			Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	45
3			Oxetane, 2,2,3-trimethyl-	100	C6H12O	023120-43-6	27
4			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	23
5			Butyric acid, 3-bromo-, methyl e...	180	C5H9BrO2	021249-59-2	23



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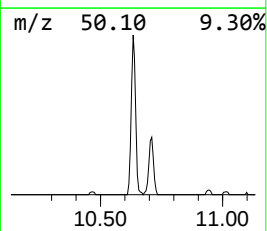
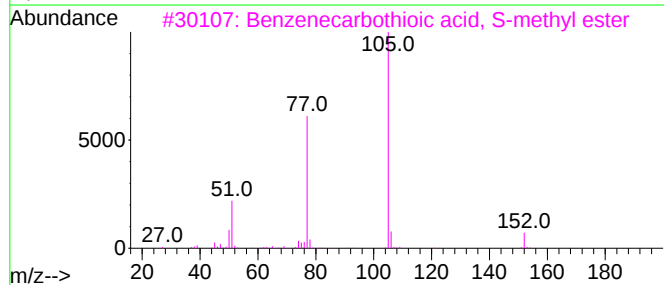
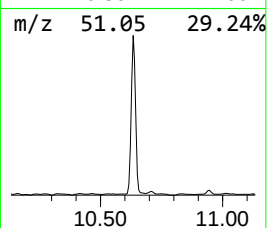
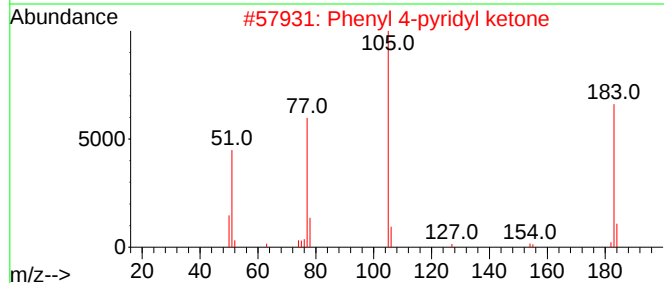
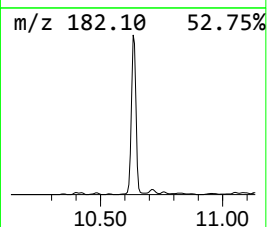
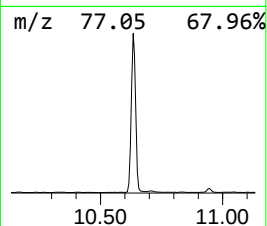
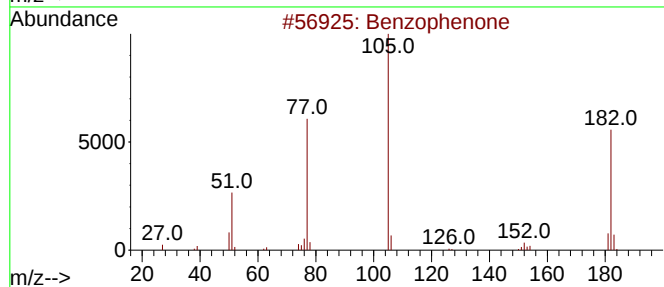
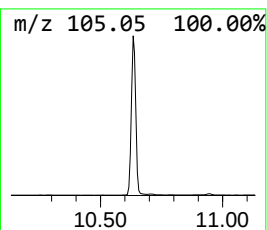
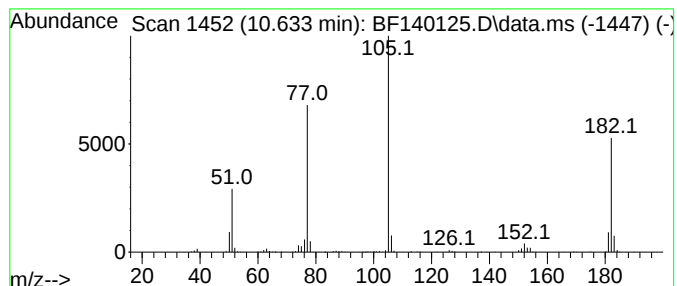
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.634	9.50 ng	501396	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	58
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
4			acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	47
5			Ethanone, 2,2,2-trifluoro-1-phenyl-	174	C8H5F3O	000434-45-7	47



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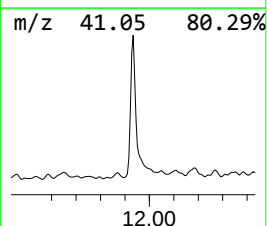
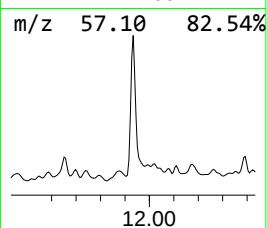
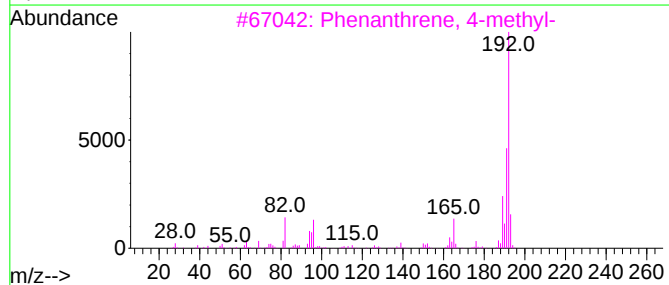
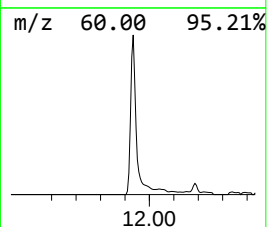
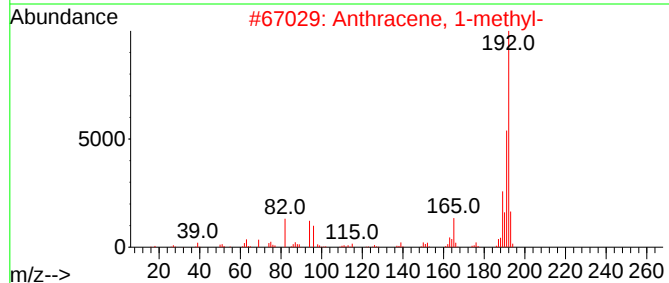
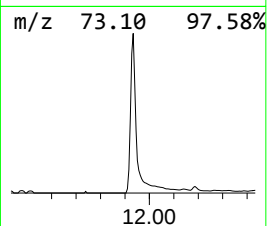
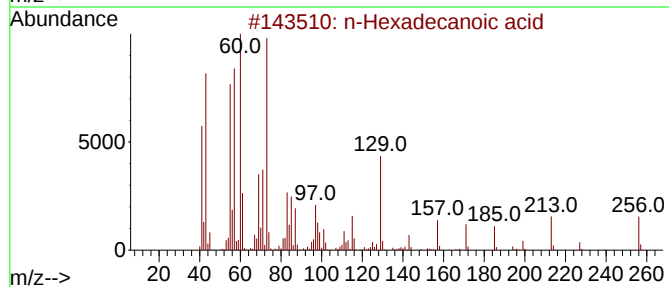
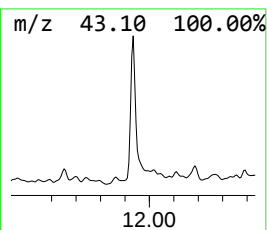
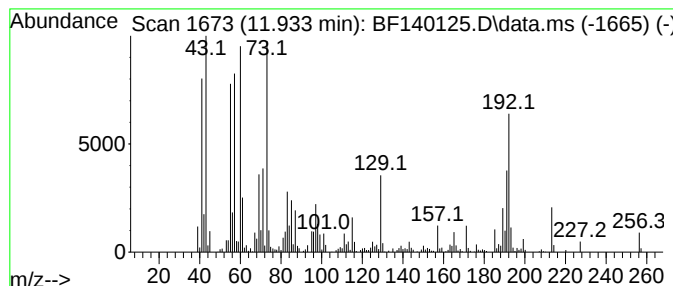
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	7.62 ng	375151	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Anthracene, 1-methyl-	192	C15H12	000610-48-0	90
3			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	90
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5			Anthracene, 2-methyl-	192	C15H12	000613-12-7	62



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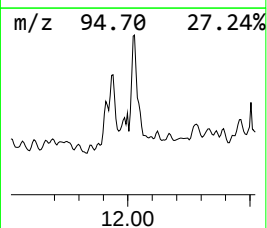
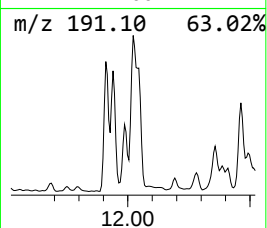
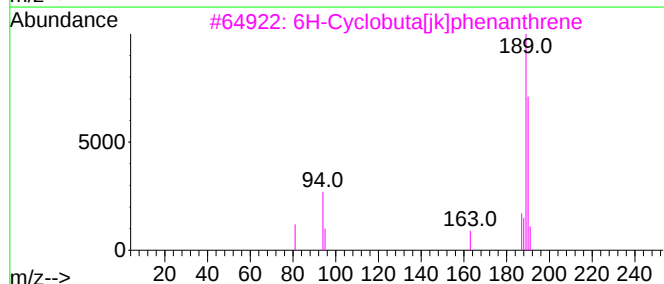
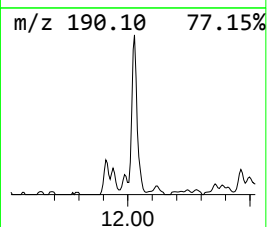
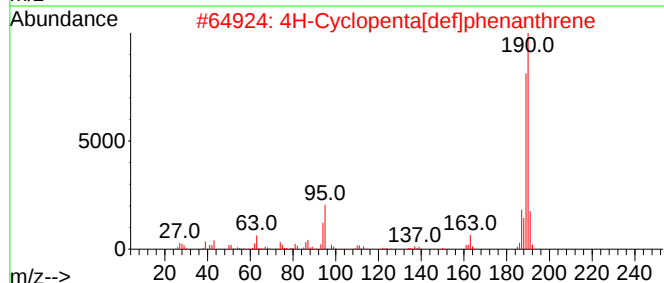
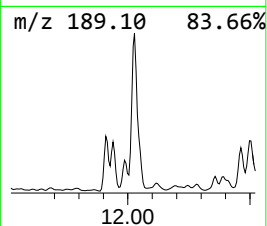
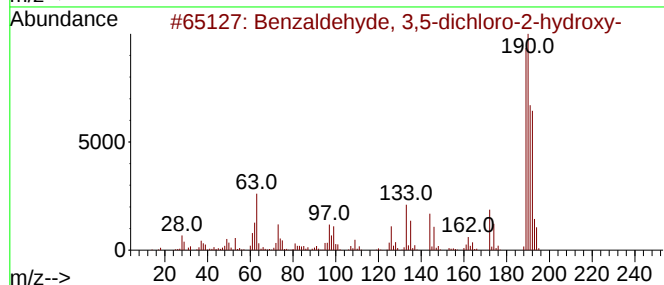
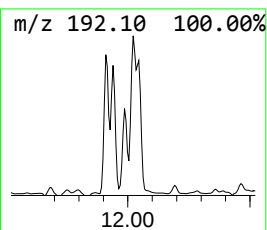
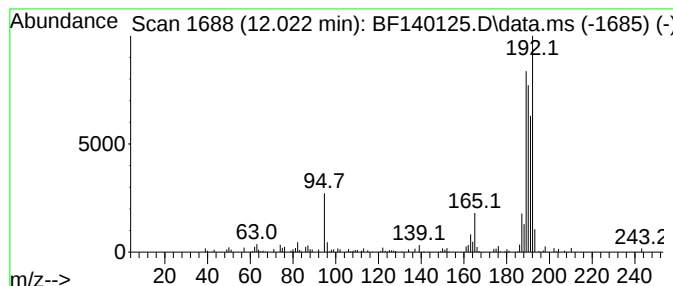
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzaldehyde, 3,5-dichloro-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.022	3.54 ng	174038	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	53
2			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	49
3			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	46
4			Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	41
5			2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102924\
Data File : BF140125.D
Acq On : 29 Oct 2024 21:13
Operator : RC/JU
Sample : P4578-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WB-305-TOP-1

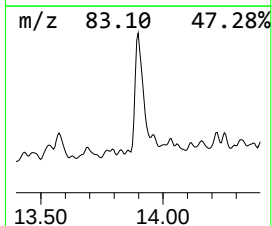
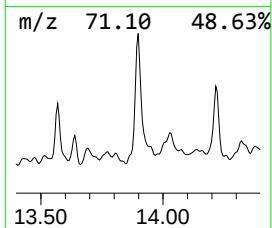
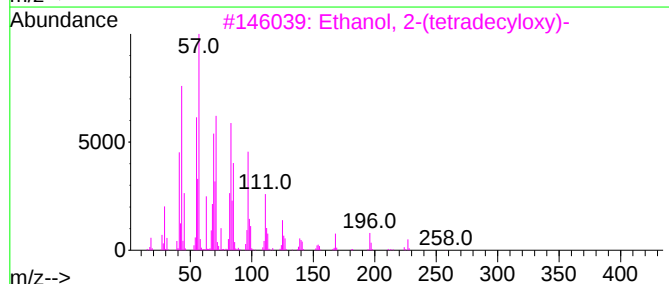
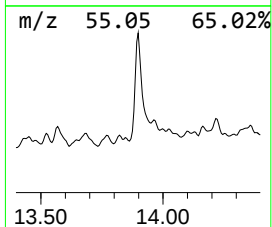
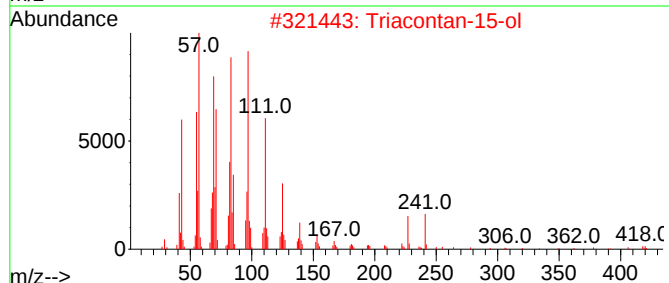
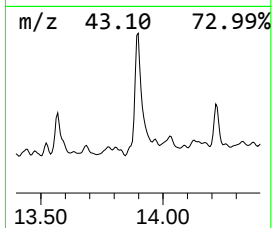
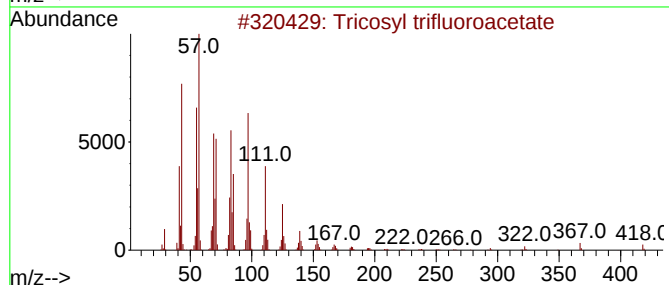
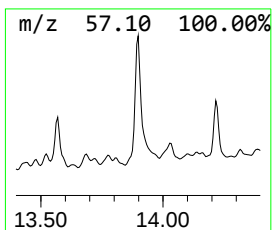
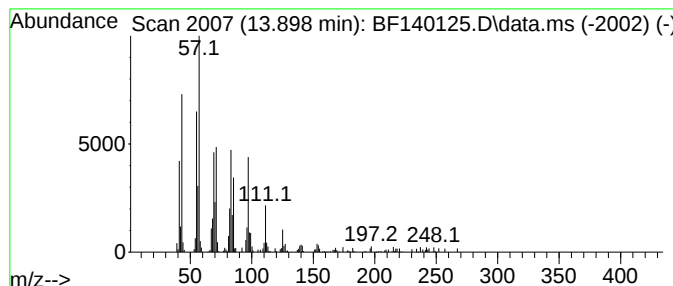
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tricosyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	3.11 ng	135355	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
2			Triacontan-15-ol	438	C30H62O	031849-26-0	91
3			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
4			Hexacosyl heptafluorobutyrate	578	C30H53F7O2	1000351-83-3	91
5			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102924\
Data File : BF140125.D
Acq On : 29 Oct 2024 21:13
Operator : RC/JU
Sample : P4578-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WB-305-TOP-1

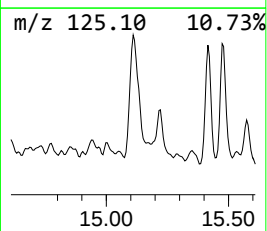
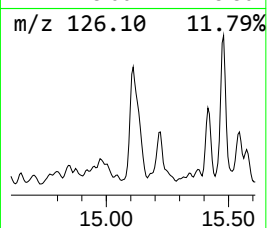
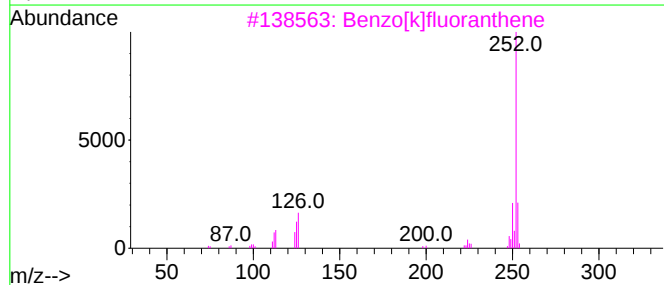
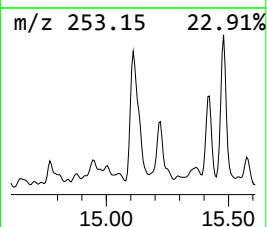
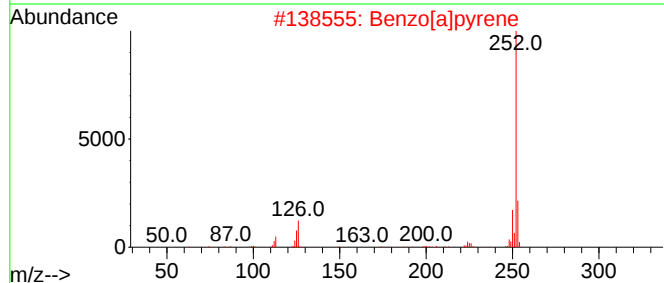
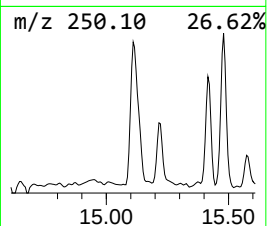
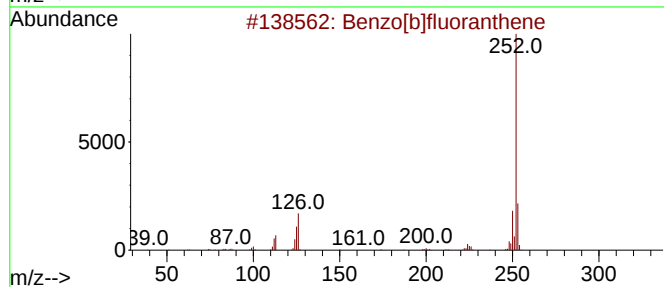
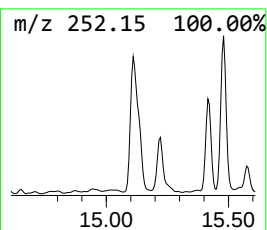
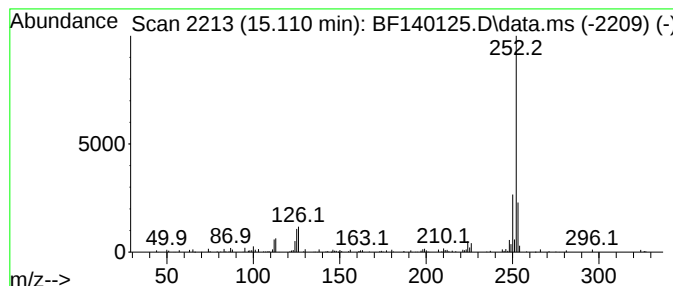
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.110	2.43 ng	81467	Perylene-d12	15.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
2			Benzo[a]pyrene	252	C20H12	000050-32-8	94
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4			Benzo[e]pyrene	252	C20H12	000192-97-2	90
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102924\
Data File : BF140125.D
Acq On : 29 Oct 2024 21:13
Operator : RC/JU
Sample : P4578-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WB-305-TOP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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...	2.193	46.6	ng	1758040	1	6.887	754398	20.0
Pentanedioic ac...	7.698	2.2	ng	117577	2	8.169	1086750	20.0
Benzophenone	10.634	9.5	ng	501396	3	9.922	1056040	20.0
n-Hexadecanoic ...	11.933	7.6	ng	375151	4	11.410	984176	20.0
Benzaldehyde, 3...	12.022	3.5	ng	174038	4	11.410	984176	20.0
Tricosyl triflu...	13.898	3.1	ng	135355	5	14.051	870255	20.0
Benzo[e]pyrene	15.110	2.4	ng	81467	6	15.545	670432	20.0