

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100924\
 Data File : BF139727.D
 Acq On : 09 Oct 2024 17:29
 Operator : RC/JU
 Sample : P4321-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 IB-6

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-BF100124.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139727.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	19	rVB	1365545	2093722	100.00%	11.399%
2	3.928	300	312	318	rBV	26574	50054	2.39%	0.273%
3	5.075	502	507	513	rVB	93250	132678	6.34%	0.722%
4	5.346	549	553	557	rBV	25230	36355	1.74%	0.198%
5	5.387	557	560	566	rVB	18485	27204	1.30%	0.148%
6	5.487	572	577	587	rVB	1158571	1548684	73.97%	8.431%
7	5.710	611	615	622	rBV	26066	35090	1.68%	0.191%
8	6.034	661	670	674	rBV	26620	41710	1.99%	0.227%
9	6.322	711	719	723	rBV	56603	87955	4.20%	0.479%
10	6.387	727	730	733	rVV	31552	41239	1.97%	0.225%
11	6.422	733	736	739	rVV	23667	27833	1.33%	0.152%
12	6.498	739	749	755	rVV	1191689	1615292	77.15%	8.794%
13	6.546	755	757	762	rVB	28430	36486	1.74%	0.199%
14	6.687	777	781	787	rBV	75583	98990	4.73%	0.539%
15	6.816	797	803	807	rVV3	12457	28221	1.35%	0.154%
16	6.863	807	811	817	rVV	408347	510372	24.38%	2.779%
17	6.922	817	821	827	rVB	22244	32074	1.53%	0.175%
18	7.046	838	842	846	rVB	68164	82305	3.93%	0.448%
19	7.110	850	853	856	rBV	39998	46594	2.23%	0.254%
20	7.181	861	865	873	rVB4	58543	112193	5.36%	0.611%
21	7.257	873	878	882	rBV	15105	25146	1.20%	0.137%
22	7.398	896	902	903	rBV	88791	108249	5.17%	0.589%
23	7.428	903	907	916	rVV	826684	1065987	50.91%	5.803%
24	7.504	916	920	924	rVV5	16479	21530	1.03%	0.117%
25	7.634	935	942	945	rBV	33930	49210	2.35%	0.268%
26	7.681	946	950	957	rVB2	21535	36782	1.76%	0.200%
27	7.745	957	961	965	rBV2	15893	22894	1.09%	0.125%
28	7.816	970	973	980	rVB3	23225	39985	1.91%	0.218%
29	7.881	980	984	988	rBV2	40485	50129	2.39%	0.273%
30	8.145	1022	1029	1036	rBV	521153	689680	32.94%	3.755%
31	8.563	1096	1100	1111	rVB2	15389	33368	1.59%	0.182%
32	9.163	1199	1202	1206	rVB	21013	25298	1.21%	0.138%
33	9.222	1206	1212	1217	rBV	1300884	1600046	76.42%	8.711%
34	9.298	1221	1225	1230	rBV3	21230	33311	1.59%	0.181%
35	9.557	1265	1269	1274	rBV3	17614	28432	1.36%	0.155%
36	9.616	1274	1279	1283	rVB3	30203	44959	2.15%	0.245%

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37	9.763	1300	1304	1307	rBV	22017	26816	1.28%	0.146%
38	9.810	1308	1312	1319	rBV3	13018	27662	1.32%	0.151%
39	9.898	1322	1327	1332	rBV	520376	664592	31.74%	3.618%
40	10.104	1358	1362	1366	rVB3	16540	24758	1.18%	0.135%
41	10.275	1387	1391	1394	rVV	53872	69383	3.31%	0.378%
42	10.310	1394	1397	1403	rVB3	18445	37355	1.78%	0.203%
43	10.445	1417	1420	1425	rVB	21368	28397	1.36%	0.155%
44	10.545	1434	1437	1442	rVB	25261	33375	1.59%	0.182%
45	10.616	1444	1449	1455	rVB	320210	414795	19.81%	2.258%
46	10.692	1457	1462	1472	rVB	666151	868028	41.46%	4.726%
47	10.810	1477	1482	1490	rVB	71298	112774	5.39%	0.614%
48	10.922	1497	1501	1507	rBV	44069	57911	2.77%	0.315%
49	11.281	1559	1562	1567	rVB2	40651	57230	2.73%	0.312%
50	11.386	1575	1580	1589	rBV2	466060	864618	41.30%	4.707%
51	11.463	1590	1593	1596	rVB	38330	45677	2.18%	0.249%
52	11.916	1662	1670	1676	rBV3	206340	359734	17.18%	1.958%
53	12.004	1681	1685	1692	rVB2	57194	112968	5.40%	0.615%
54	12.604	1783	1787	1791	rBV	368255	455584	21.76%	2.480%
55	12.698	1800	1803	1810	rBV4	45133	62615	2.99%	0.341%
56	12.833	1820	1826	1831	rVB	304451	445731	21.29%	2.427%
57	12.969	1844	1849	1857	rVB	806617	1095287	52.31%	5.963%
58	14.027	2023	2029	2033	rBV2	478652	827131	39.51%	4.503%
59	15.074	2202	2207	2214	rBV	180971	385632	18.42%	2.099%
60	15.439	2265	2269	2275	rVB	146569	214979	10.27%	1.170%
61	15.504	2275	2280	2295	rVB2	292837	515246	24.61%	2.805%

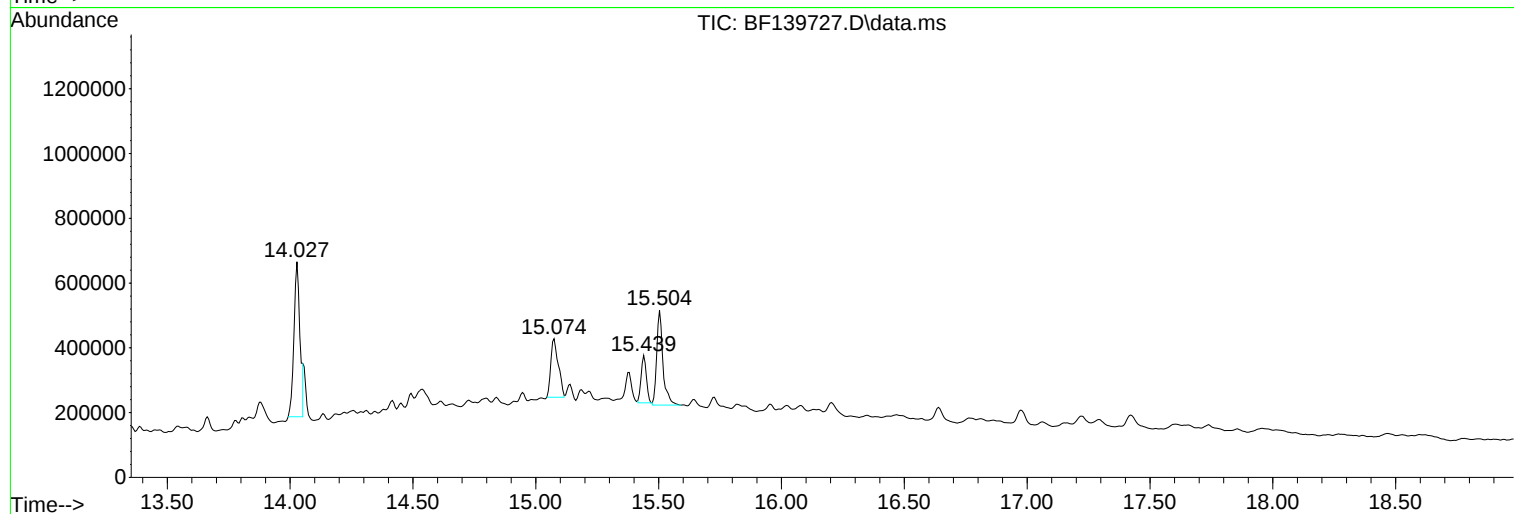
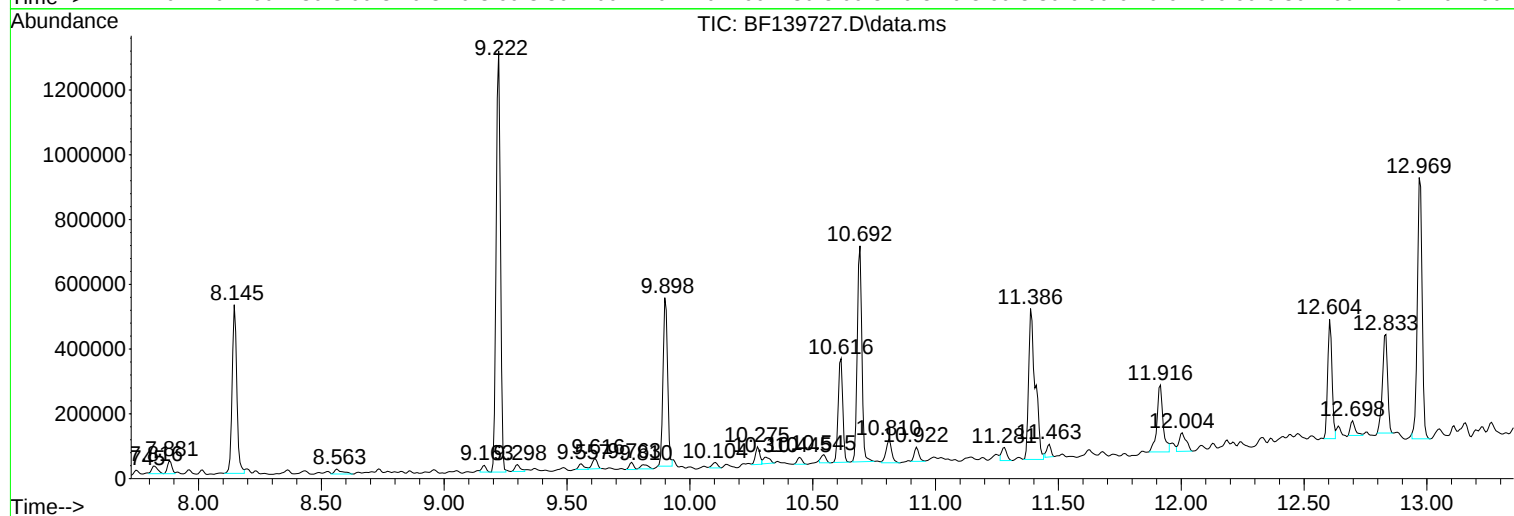
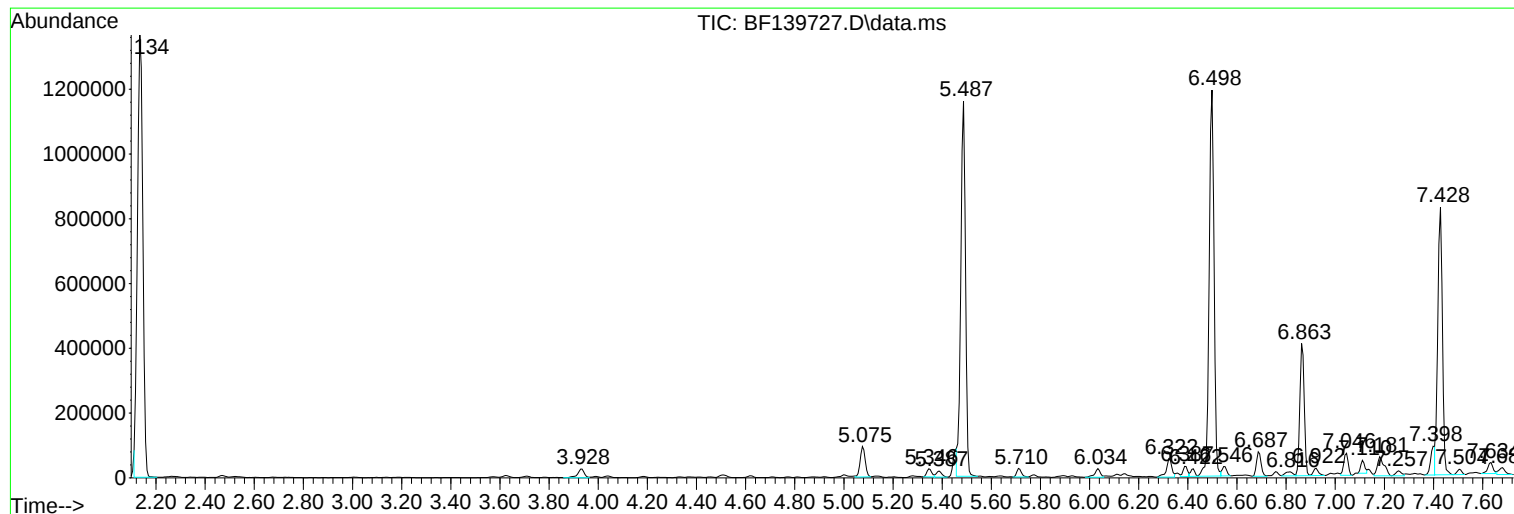
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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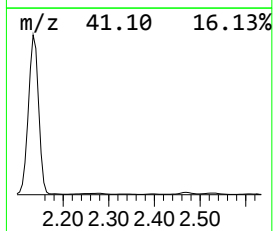
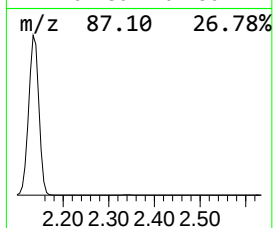
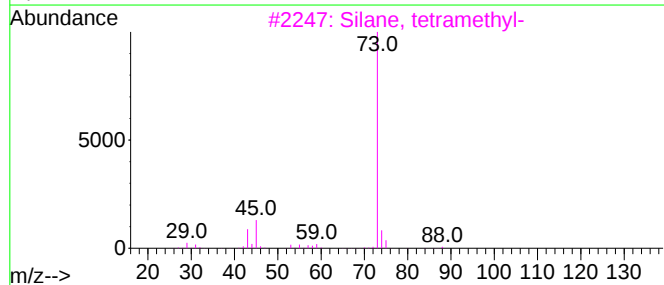
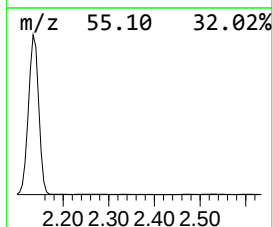
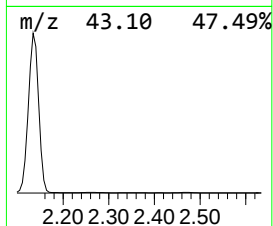
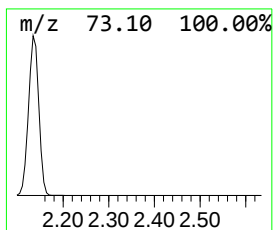
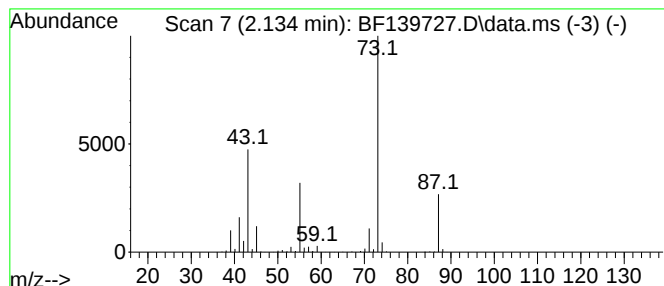
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.134	82.05 ng	2093720	1,4-Dichlorobenzene-d4	6.863

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			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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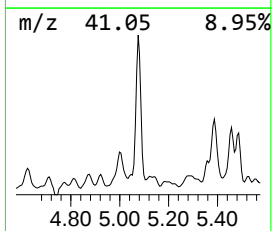
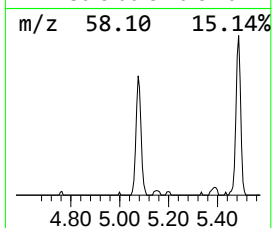
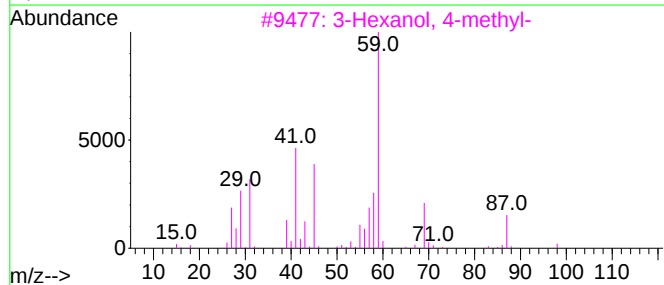
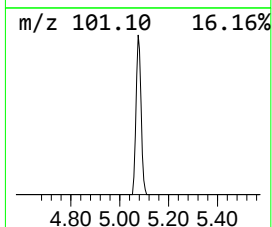
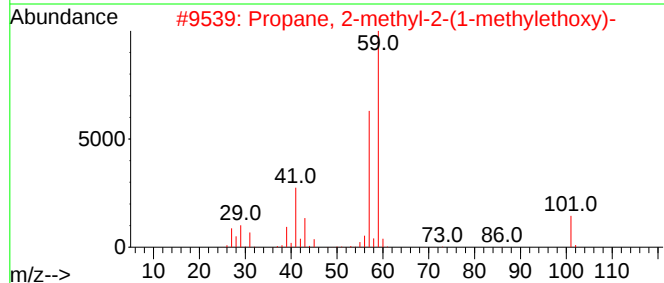
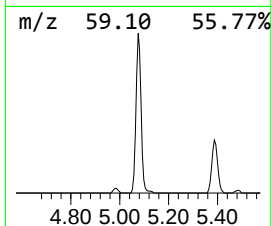
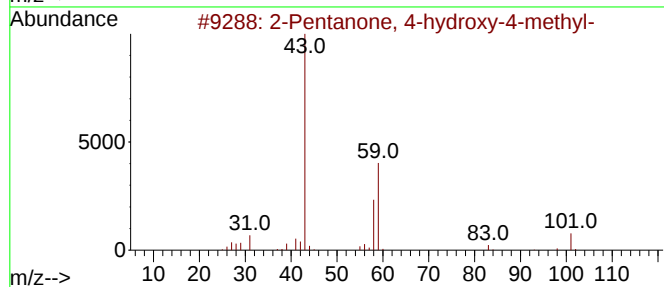
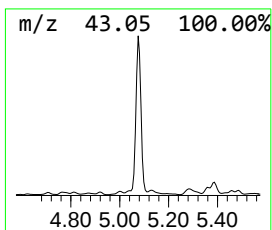
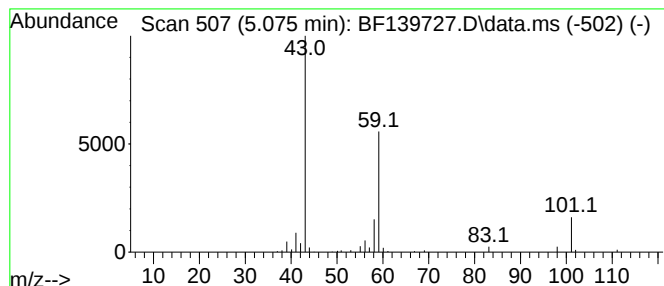
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	5.20 ng	132678	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
4	3-Octanol	130	C8H18O	000589-98-0	33		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		



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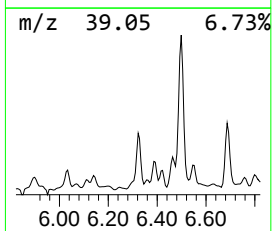
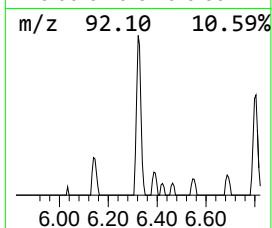
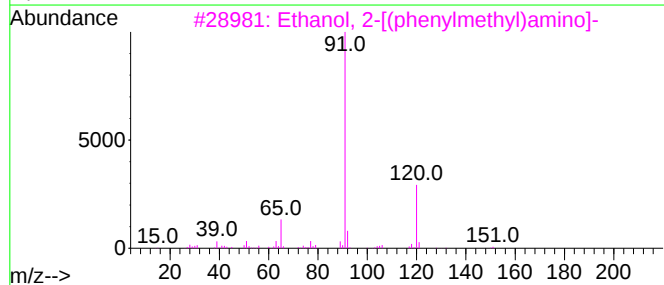
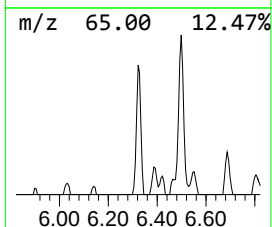
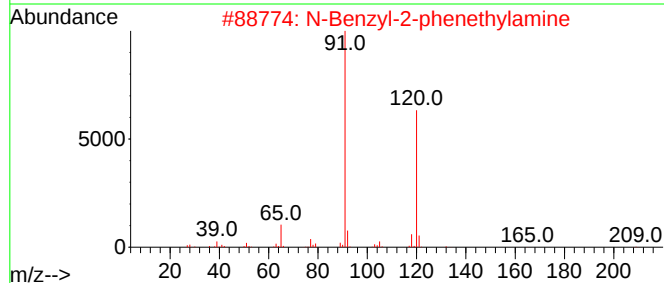
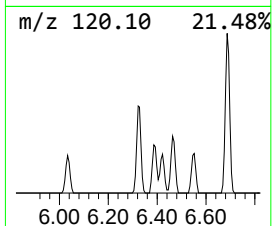
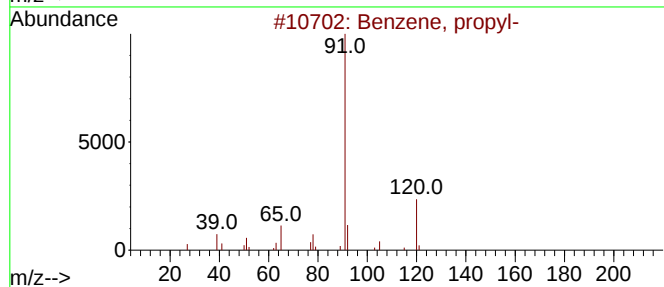
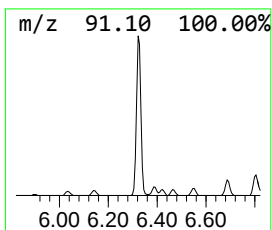
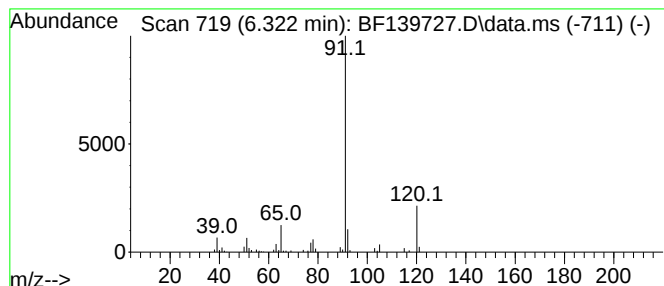
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzene, propyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.322	3.45 ng	87955	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, propyl-	120	C9H12	000103-65-1	94
2			N-Benzyl-2-phenethylamine	211	C15H17N	003647-71-0	78
3			Ethanol, 2-[(phenylmethyl)amino]-	151	C9H13NO	000104-63-2	72
4			Phenethylamine, N-benzyl-p-chloro-	245	C15H16ClN	013622-43-0	72
5			N-(Cyclohexylmethyl)(phenyl)meth...	203	C14H21N	004352-47-0	72



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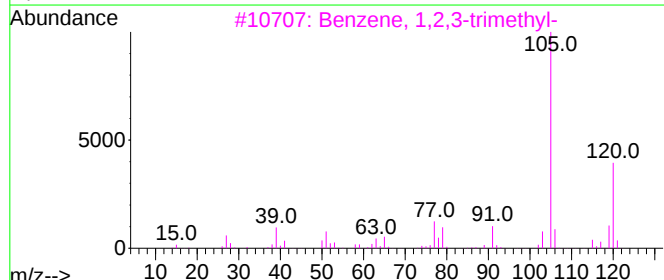
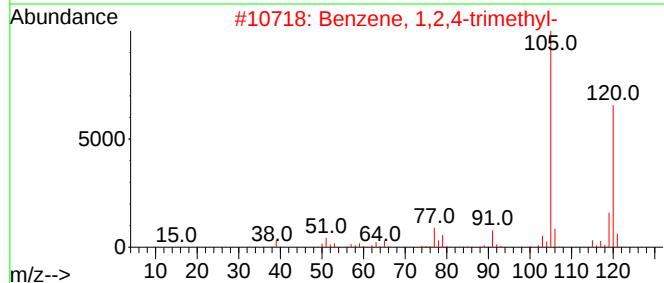
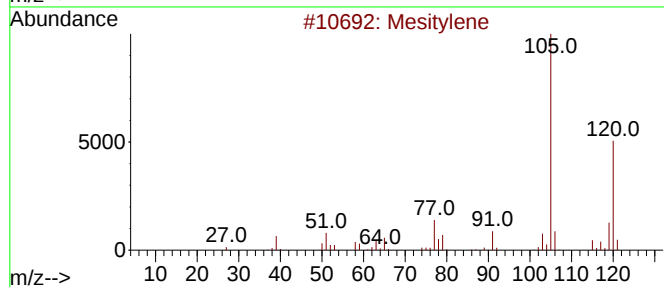
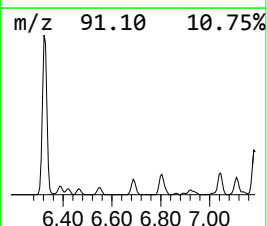
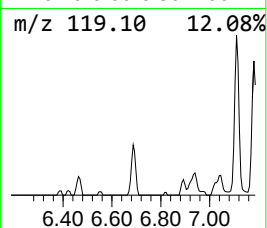
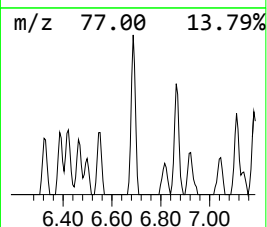
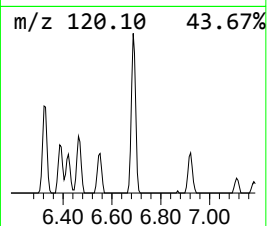
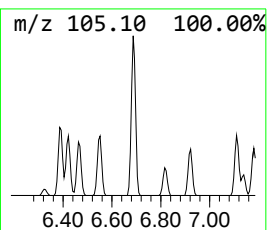
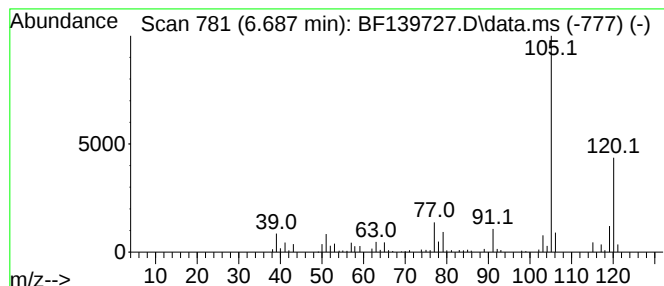
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Mesitylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.687	3.88 ng	98990	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	97
2			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	95
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	94
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



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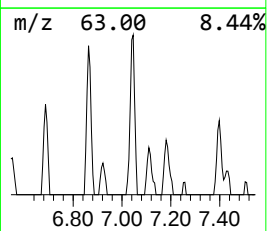
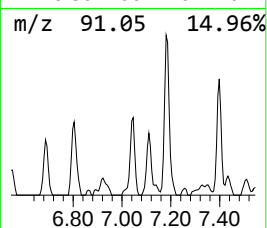
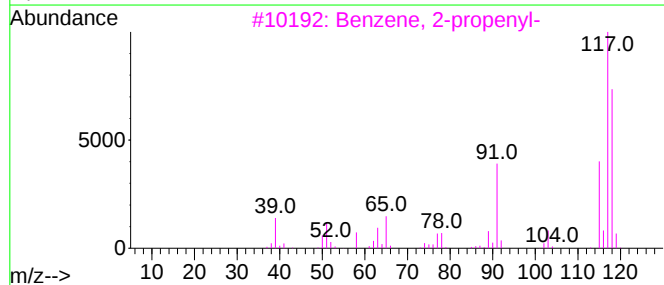
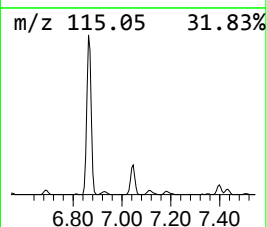
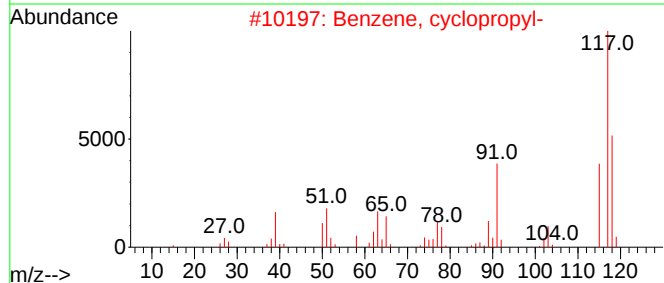
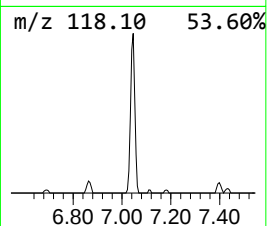
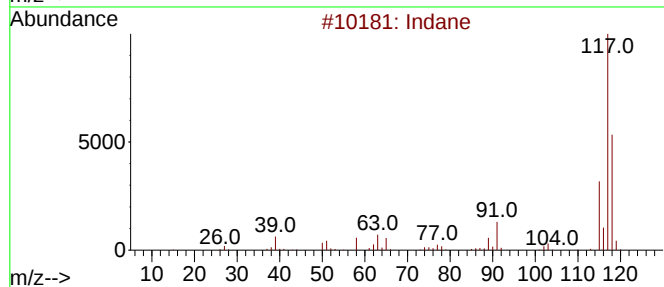
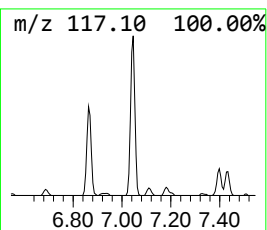
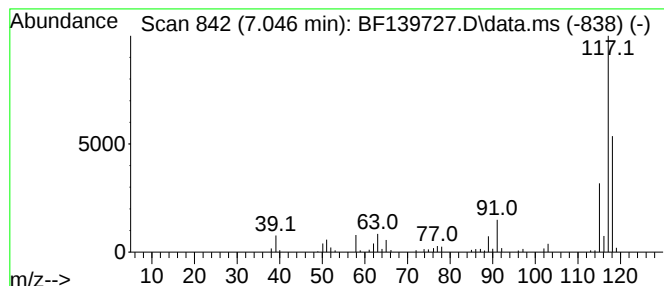
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Indane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.046	3.23 ng	82305	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	91
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	72
4			Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59
5			trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100924\
Data File : BF139727.D
Acq On : 09 Oct 2024 17:29
Operator : RC/JU
Sample : P4321-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
IB-6

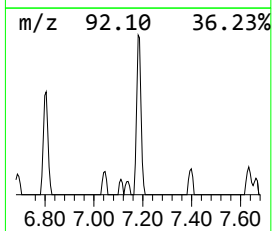
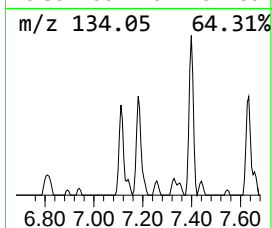
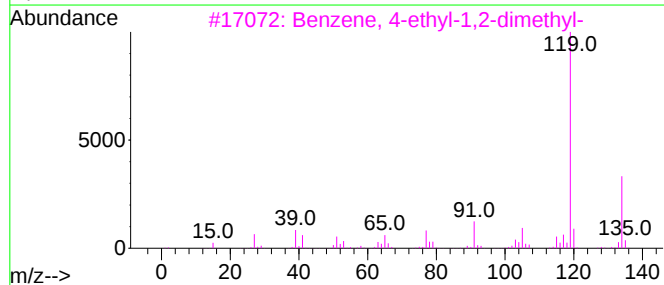
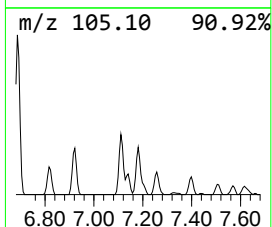
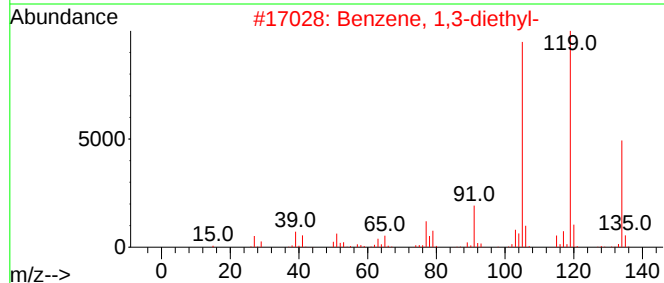
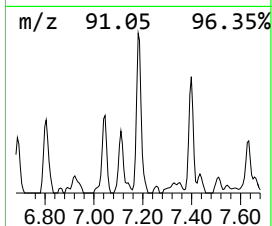
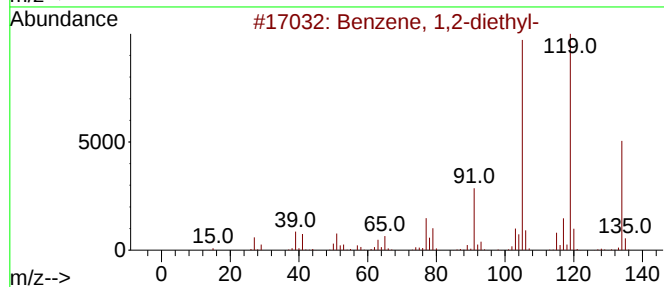
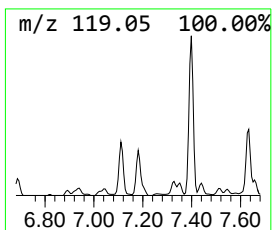
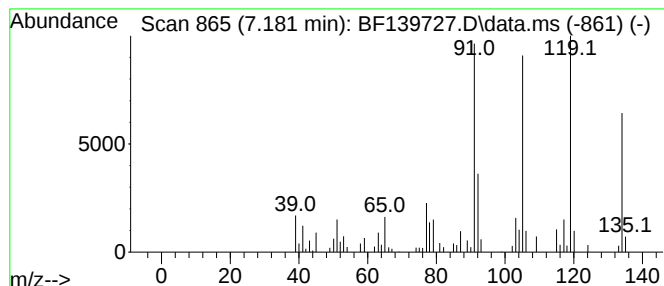
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzene, 1,2-diethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.181	4.40 ng	112193	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	93
2			Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	93
3			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	90
4			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	90
5			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100924\
Data File : BF139727.D
Acq On : 09 Oct 2024 17:29
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Sample : P4321-01
Misc :
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Instrument :
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ClientSampleId :
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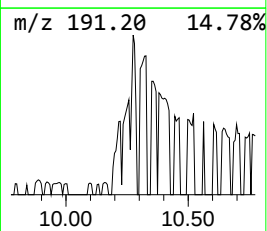
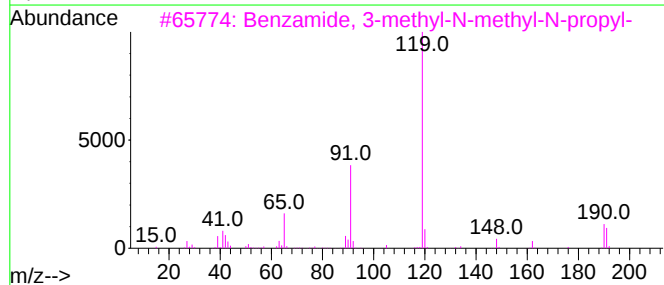
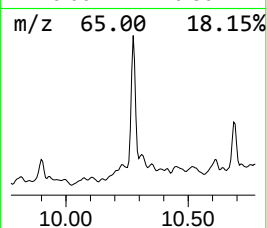
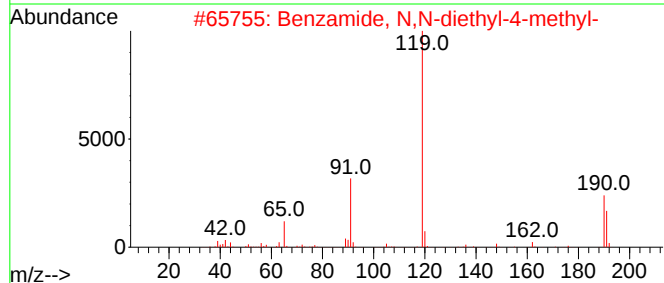
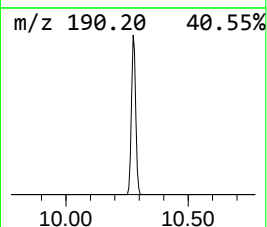
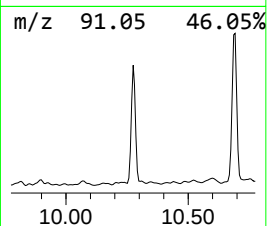
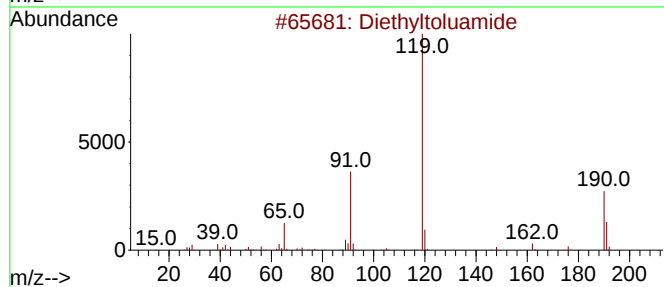
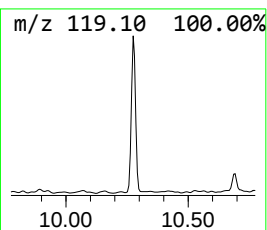
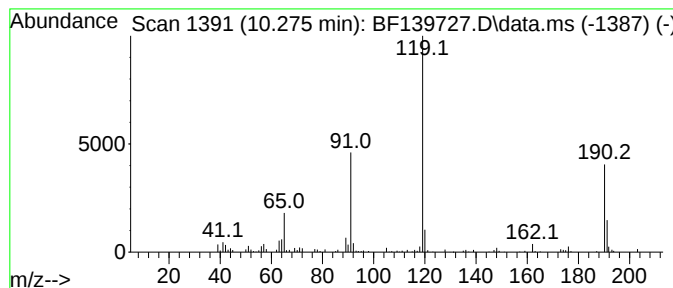
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Diethyltoluamide Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.275	2.09 ng	69383	Acenaphthene-d10	9.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethyltoluamide	191	C12H17NO	000134-62-3	96
2			Benzamide, N,N-diethyl-4-methyl-	191	C12H17NO	002728-05-4	87
3			Benzamide, 3-methyl-N-methyl-N-p...	191	C12H17NO	1000421-46-2	81
4			Benzamide, 4-methyl-N-butyl-	191	C12H17NO	1000407-46-6	76
5			Benzamide, 3-methyl-N-butyl-	191	C12H17NO	1000407-41-1	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100924\
Data File : BF139727.D
Acq On : 09 Oct 2024 17:29
Operator : RC/JU
Sample : P4321-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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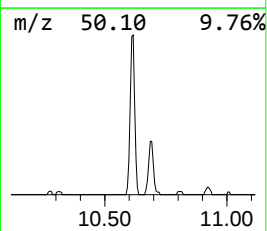
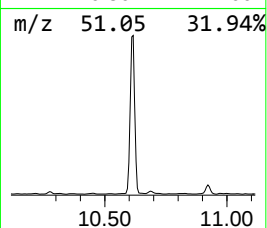
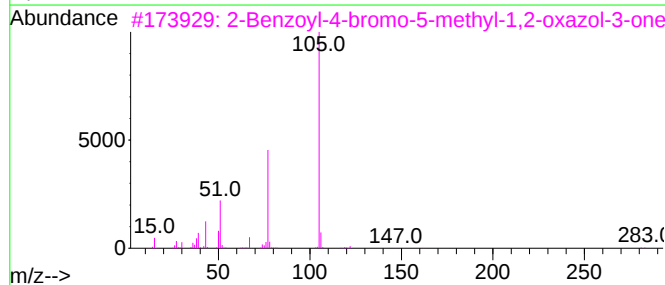
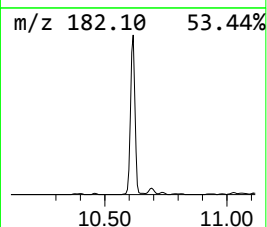
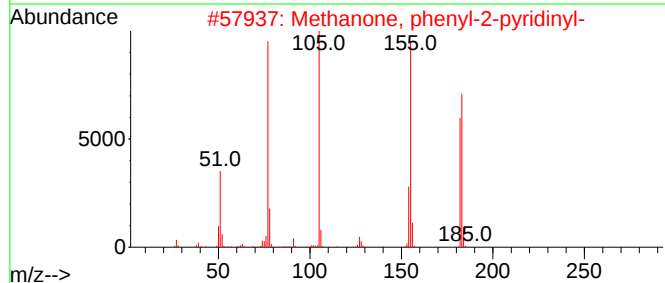
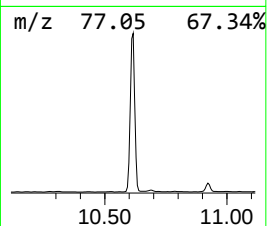
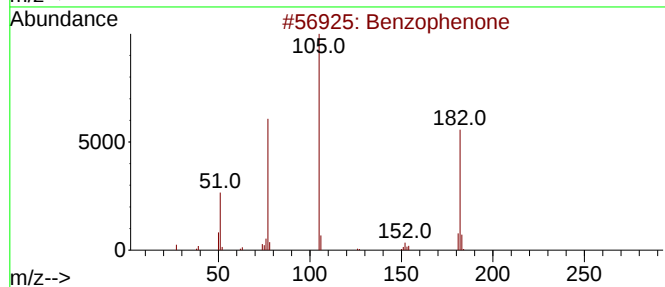
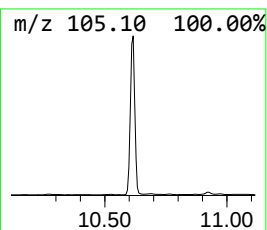
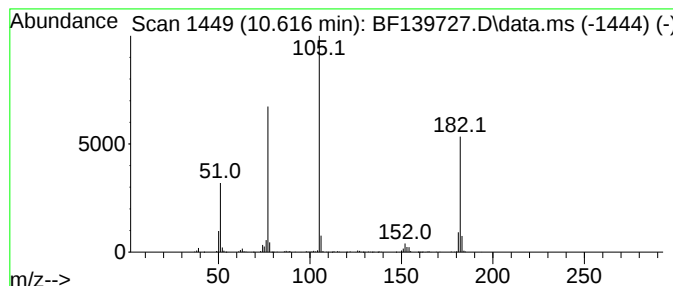
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.616	12.48 ng	414795	Acenaphthene-d10	9.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	72
3			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47
4			2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	47
5			Isopropyl phenyl ketone	148	C10H12O	000611-70-1	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100924\
Data File : BF139727.D
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Operator : RC/JU
Sample : P4321-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

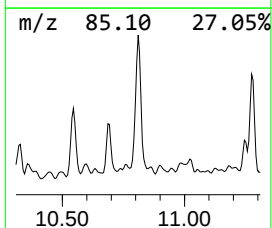
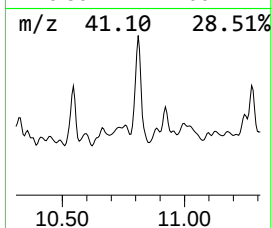
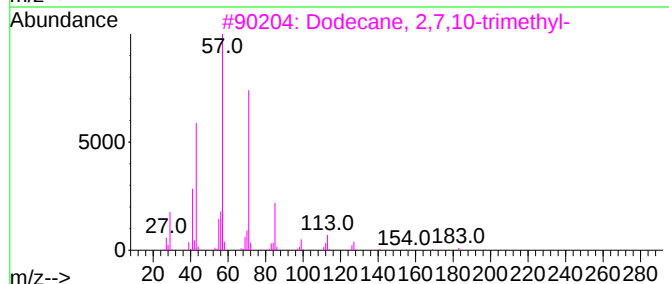
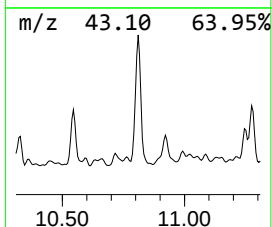
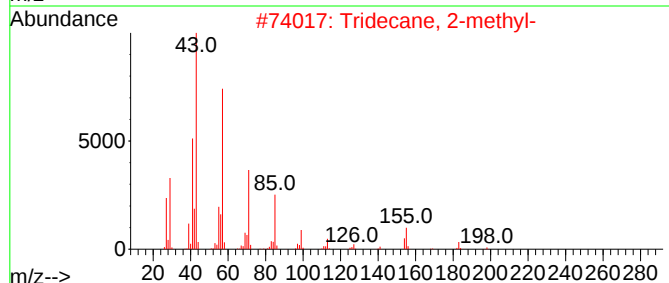
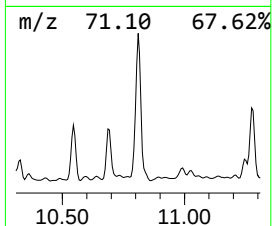
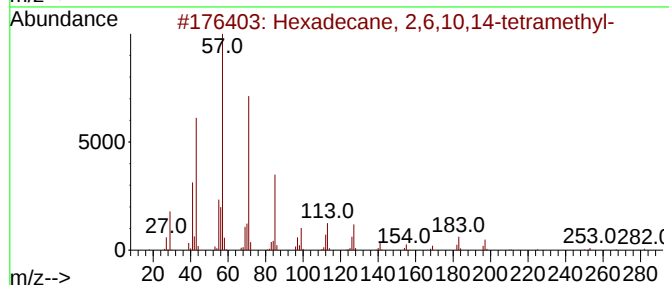
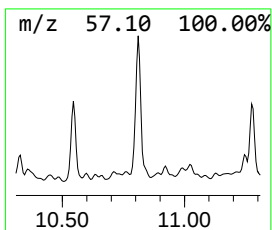
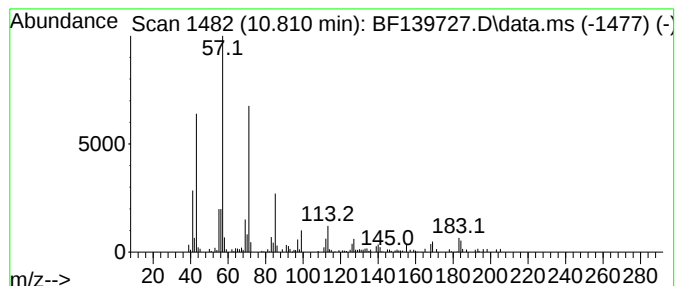
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecane, 2,6,10,14-tetra... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD			R.T.
10.810	2.61 ng	112774	Phenanthrene-d10			11.386
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-		282	C20H42	000638-36-8	86
2	Tridecane, 2-methyl-		198	C14H30	001560-96-9	80
3	Dodecane, 2,7,10-trimethyl-		212	C15H32	074645-98-0	80
4	Tridecane		184	C13H28	000629-50-5	68
5	Nonane, 3,7-dimethyl-		156	C11H24	017302-32-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100924\
Data File : BF139727.D
Acq On : 09 Oct 2024 17:29
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Sample : P4321-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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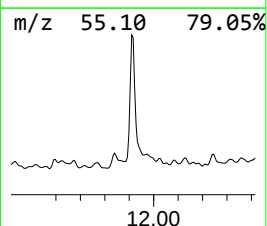
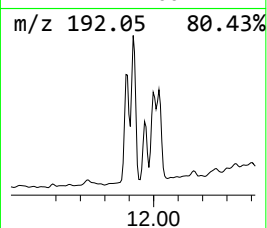
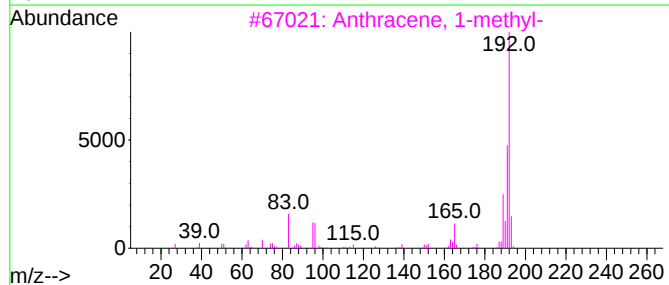
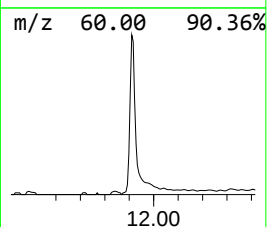
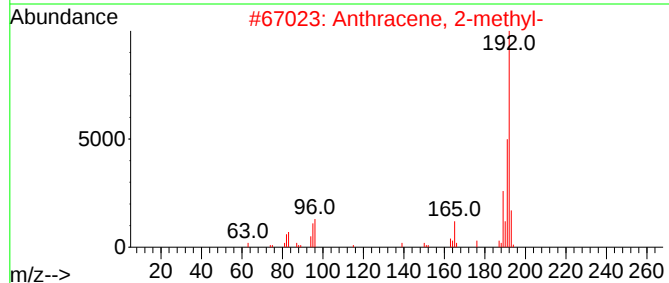
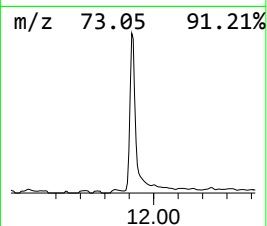
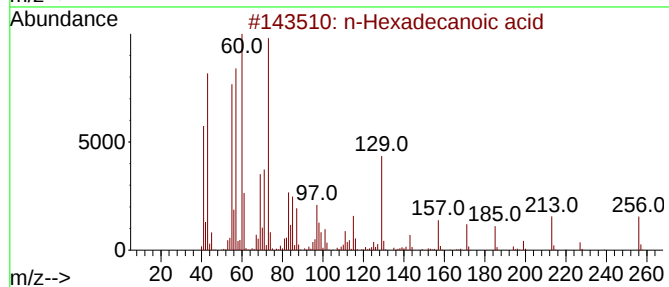
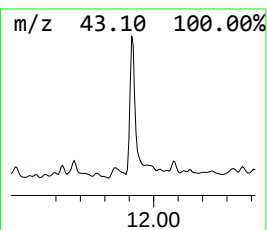
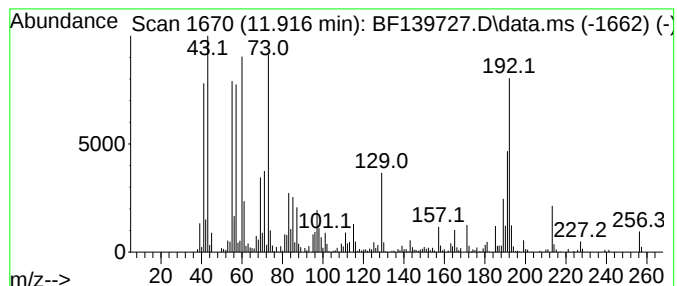
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	8.32 ng	359734	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Anthracene, 2-methyl-	192	C15H12	000613-12-7	94
3			Anthracene, 1-methyl-	192	C15H12	000610-48-0	92
4			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	92
5			Anthracene, 9-methyl-	192	C15H12	000779-02-2	92



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100924\
Data File : BF139727.D
Acq On : 09 Oct 2024 17:29
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Misc :
ALS Vial : 17 Sample Multiplier: 1

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ClientSampleId :
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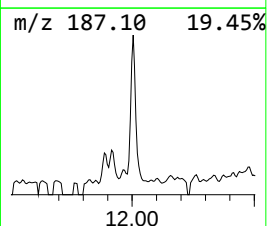
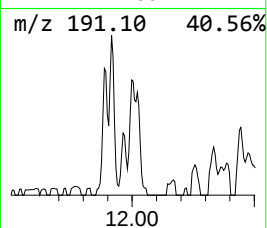
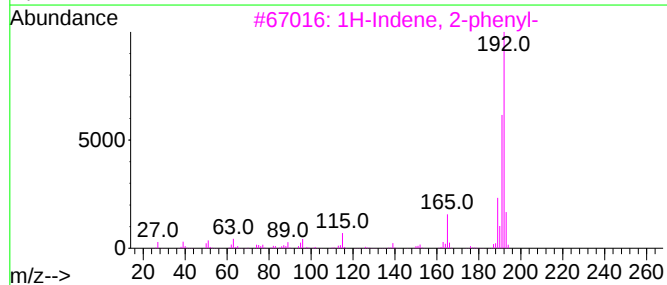
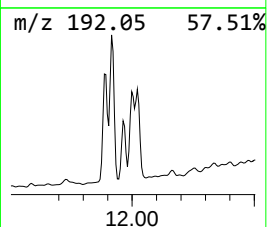
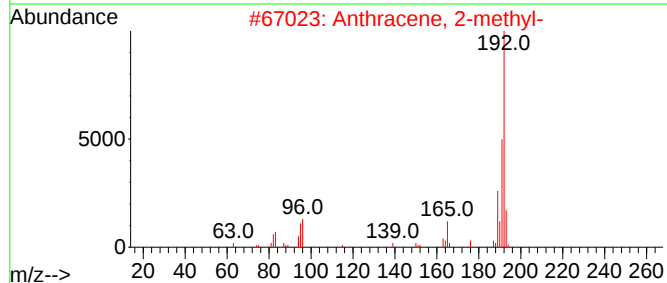
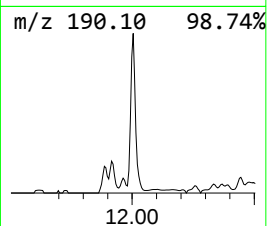
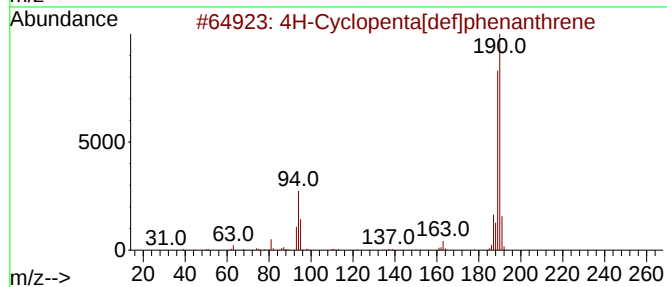
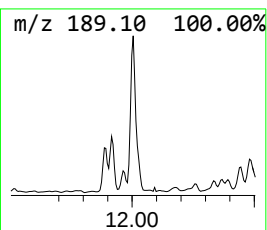
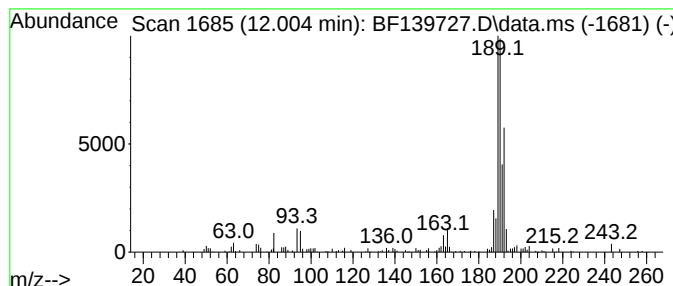
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 4H-Cyclopenta[def]phenanthrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.004	2.61 ng	112968	Phenanthrene-d10	11.386

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2		Anthracene, 2-methyl-	192	C15H12	000613-12-7	38
3		1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	30
4		Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	30
5		Propyne, 1,3-diphenyl-	192	C15H12	004980-70-5	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100924\
Data File : BF139727.D
Acq On : 09 Oct 2024 17:29
Operator : RC/JU
Sample : P4321-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
IB-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.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	82.0	ng	2093720	1	6.863	510372	20.0
2-Pentanone, 4-...	5.075	5.2	ng	132678	1	6.863	510372	20.0
Benzene, propyl-	6.322	3.5	ng	87955	1	6.863	510372	20.0
Mesitylene	6.687	3.9	ng	98990	1	6.863	510372	20.0
Indane	7.046	3.2	ng	82305	1	6.863	510372	20.0
Benzene, 1,2-di...	7.181	4.4	ng	112193	1	6.863	510372	20.0
Diethyltoluamide	10.275	2.1	ng	69383	3	9.898	664592	20.0
Benzophenone	10.616	12.5	ng	414795	3	9.898	664592	20.0
Hexadecane, 2,6...	10.810	2.6	ng	112774	4	11.386	864618	20.0
n-Hexadecanoic ...	11.916	8.3	ng	359734	4	11.386	864618	20.0
4H-Cyclopenta[d...	12.004	2.6	ng	112968	4	11.386	864618	20.0