

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100924\
 Data File : BF139735.D
 Acq On : 09 Oct 2024 21:21
 Operator : RC/JU
 Sample : P4353-01
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CF-400-COMP-43

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: BF139735.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	17	rVB	1755651	2764945	100.00%	15.007%
2	2.481	57	66	74	rVB	16247	39689	1.44%	0.215%
3	5.081	503	508	517	rVB	86820	129102	4.67%	0.701%
4	5.487	568	577	597	rBV	1275070	1746253	63.16%	9.478%
5	6.498	743	749	764	rBV	1315543	1781331	64.43%	9.668%
6	6.869	807	812	817	rVB	388948	488521	17.67%	2.652%
7	7.428	898	907	912	rBV	885764	1134342	41.03%	6.157%
8	7.681	945	950	955	rBV	39227	51629	1.87%	0.280%
9	8.145	1024	1029	1041	rVB	471773	618612	22.37%	3.358%
10	9.222	1207	1212	1217	rBV	1563656	1911401	69.13%	10.374%
11	9.628	1276	1281	1286	rVB	18706	29239	1.06%	0.159%
12	9.763	1300	1304	1310	rBV	72730	88593	3.20%	0.481%
13	9.904	1321	1328	1333	rBV	453792	592559	21.43%	3.216%
14	10.616	1443	1449	1456	rBV	146341	192254	6.95%	1.043%
15	10.692	1456	1462	1477	rVV	689456	902260	32.63%	4.897%
16	11.386	1575	1580	1590	rBV	402335	589868	21.33%	3.202%
17	11.463	1590	1593	1596	rBV	24628	28220	1.02%	0.153%
18	11.916	1661	1670	1676	rBV2	257235	445890	16.13%	2.420%
19	12.004	1681	1685	1693	rVB	63589	141712	5.13%	0.769%
20	12.186	1709	1716	1718	rBV4	22850	42226	1.53%	0.229%
21	12.333	1735	1741	1744	rBV3	15647	34326	1.24%	0.186%
22	12.439	1754	1759	1762	rBV	73311	107929	3.90%	0.586%
23	12.474	1762	1765	1771	rVV2	43008	83025	3.00%	0.451%
24	12.527	1771	1774	1778	rVV2	32167	43483	1.57%	0.236%
25	12.604	1782	1787	1791	rBV	130532	170635	6.17%	0.926%
26	12.698	1799	1803	1807	rBV	81128	102009	3.69%	0.554%
27	12.833	1821	1826	1832	rBV	189449	274977	9.95%	1.492%
28	12.886	1832	1835	1839	rVB2	29868	38289	1.38%	0.208%
29	12.974	1845	1850	1857	rVB	1213468	1556790	56.30%	8.450%
30	13.051	1859	1863	1869	rBV4	54946	100170	3.62%	0.544%
31	13.145	1874	1879	1885	rVB2	59937	135479	4.90%	0.735%
32	13.204	1886	1889	1891	rBV3	20562	29483	1.07%	0.160%
33	13.263	1896	1899	1903	rVB2	57884	73347	2.65%	0.398%
34	13.357	1911	1915	1918	rBV	61701	79015	2.86%	0.429%
35	13.386	1918	1920	1924	rVB2	51257	55893	2.02%	0.303%
36	13.880	2000	2004	2013	rVB2	84540	174734	6.32%	0.948%

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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-BF100124.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.033	2024	2030	2041	rVB3	438956	805448	29.13%	4.372%
38	14.416	2092	2095	2099	rBV	57793	74847	2.71%	0.406%
39	14.786	2154	2158	2164	rVB	175969	244158	8.83%	1.325%
40	15.074	2204	2207	2214	rVB	78901	141003	5.10%	0.765%
41	15.510	2276	2281	2293	rVB	218749	380454	13.76%	2.065%

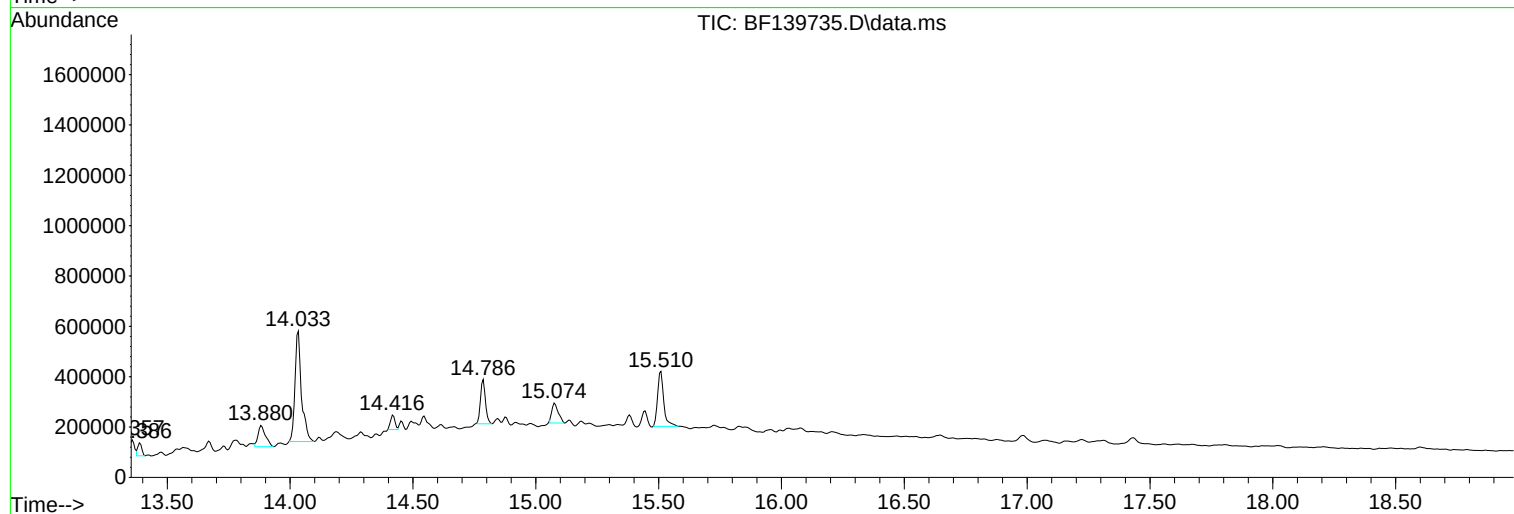
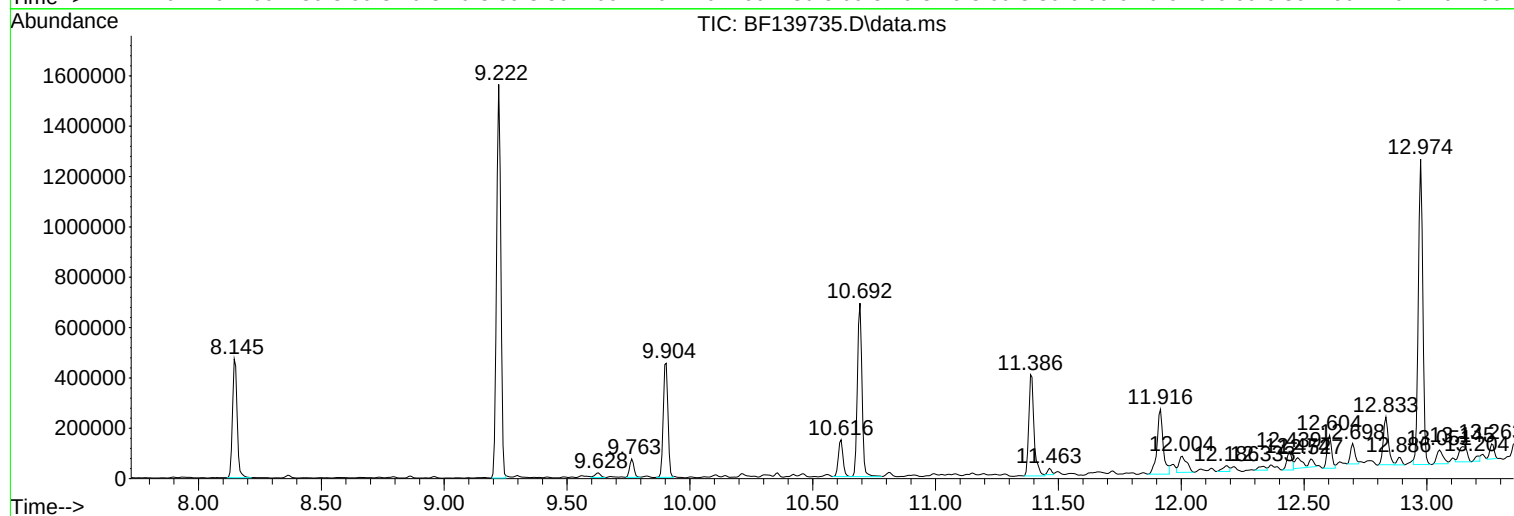
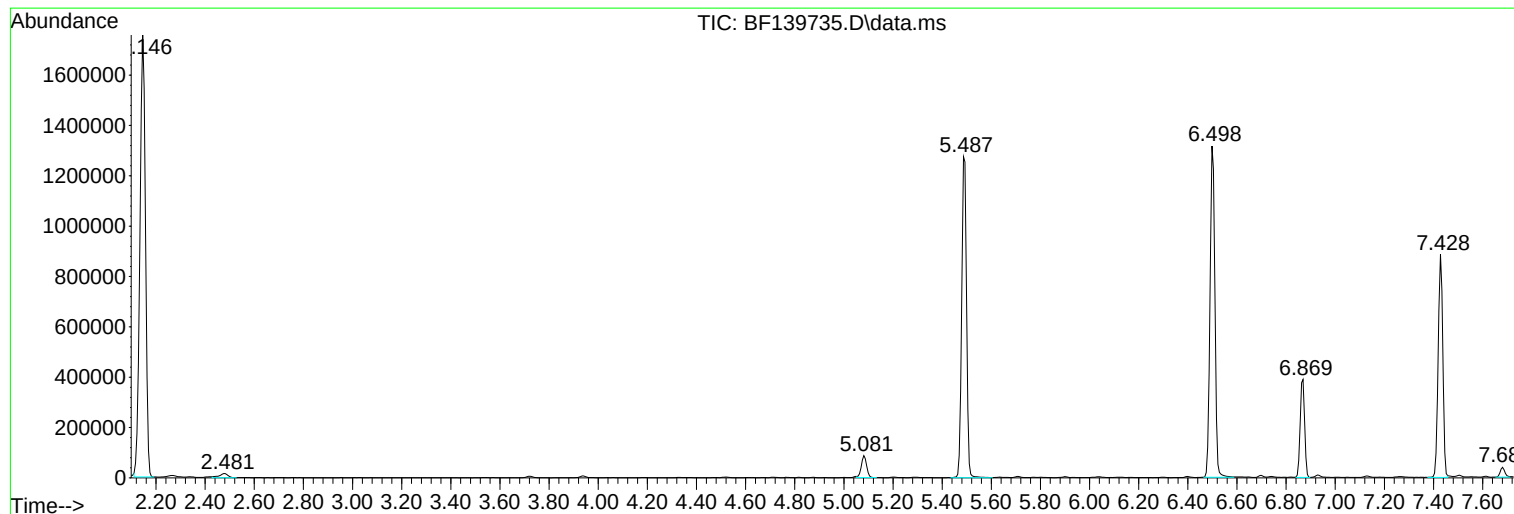
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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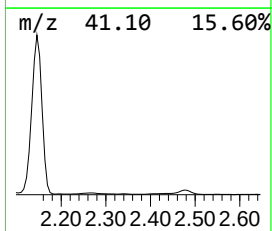
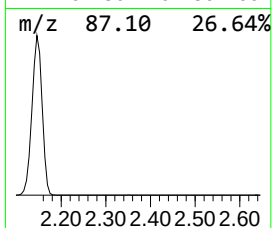
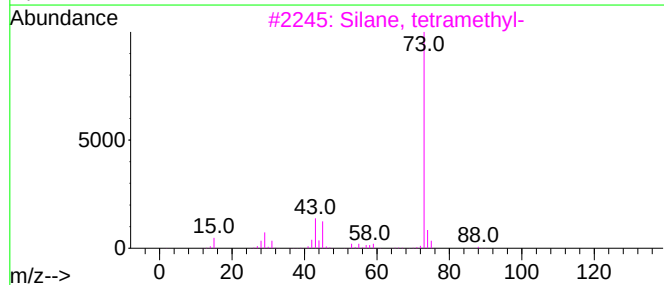
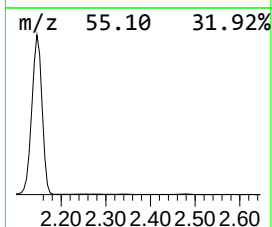
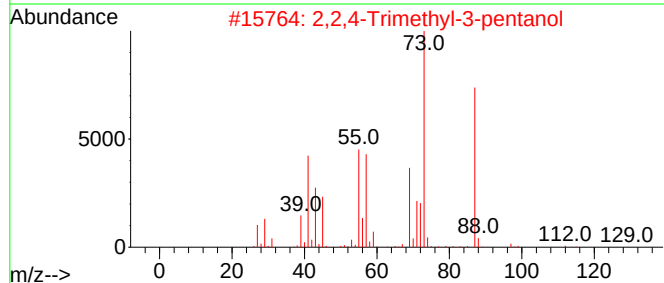
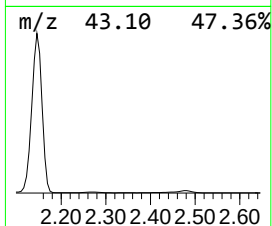
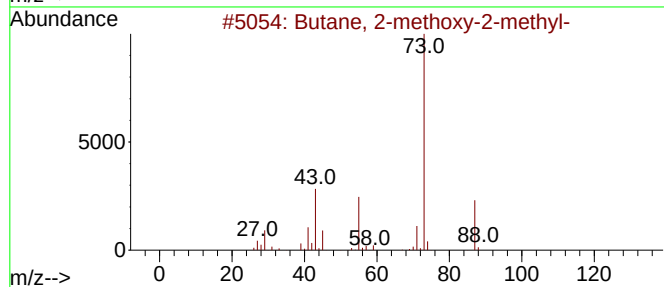
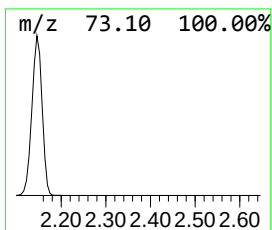
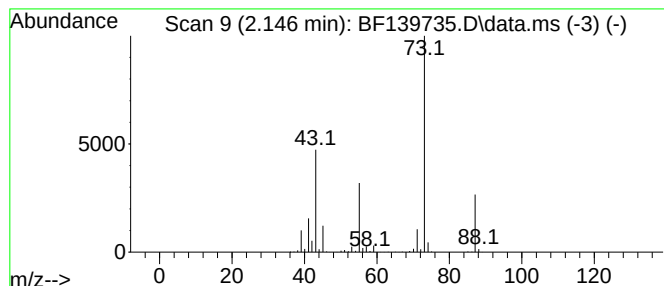
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.146	113.20 ng	2764950	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	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			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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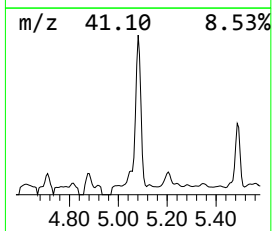
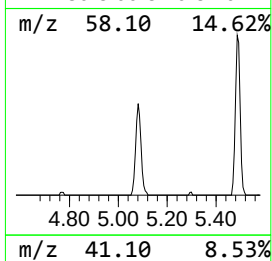
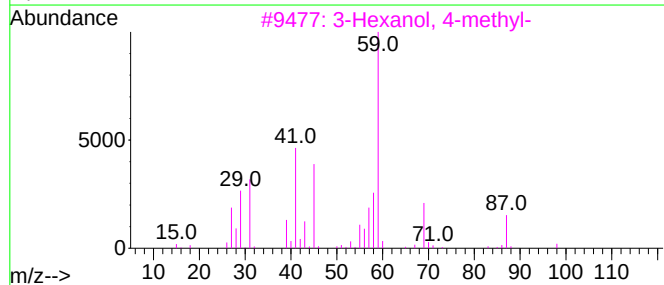
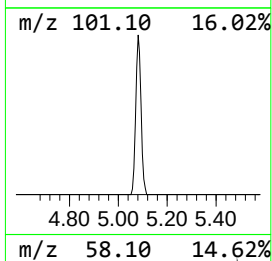
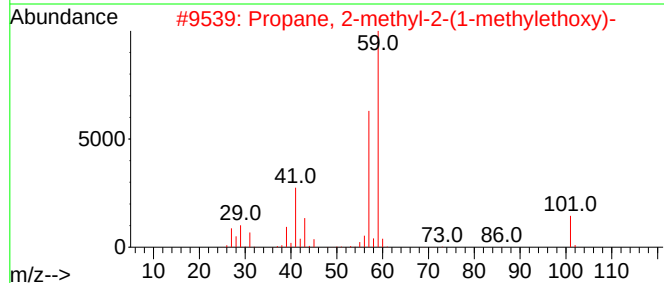
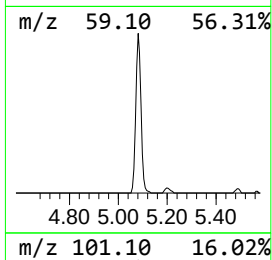
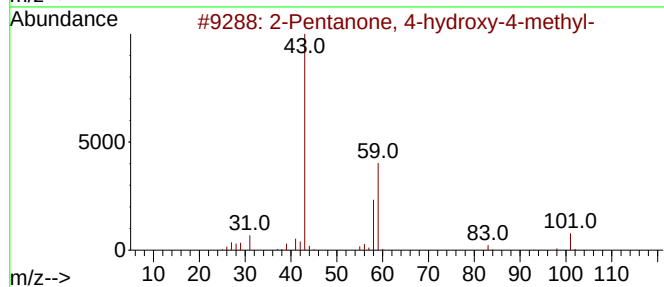
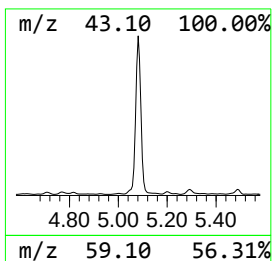
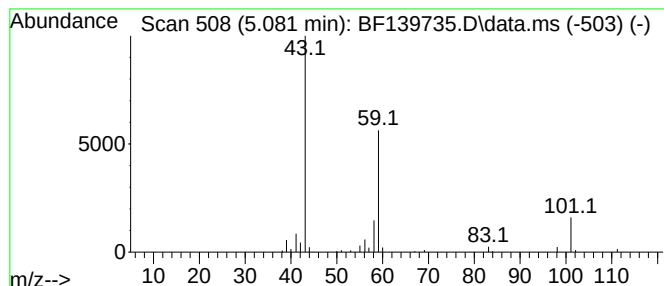
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.081	5.29 ng	129102	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	50
2	Propane, 2-methyl-2-(1-methyleth...		116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-		116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	23
5	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	12



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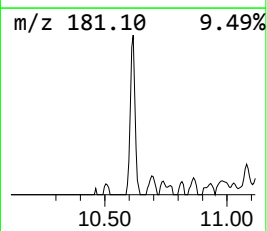
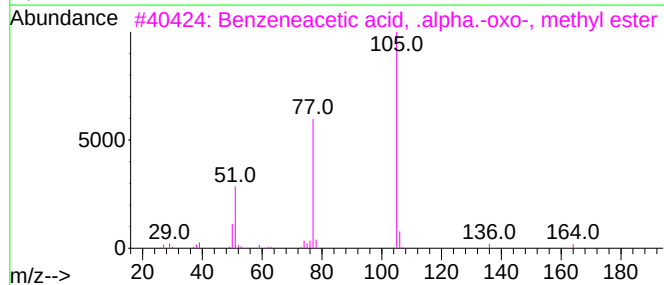
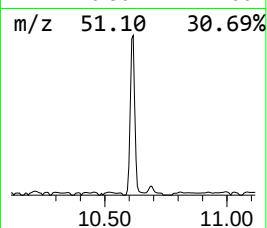
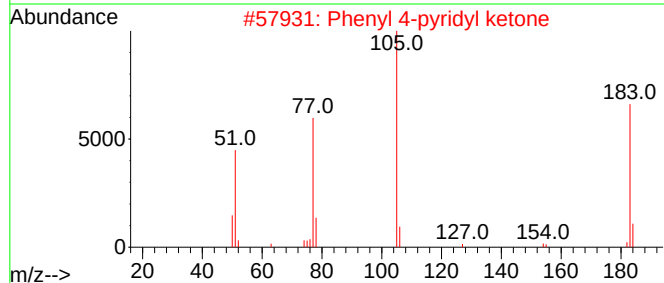
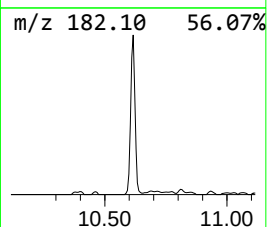
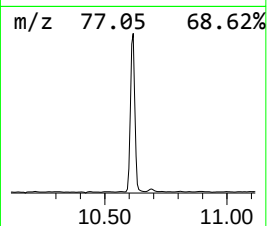
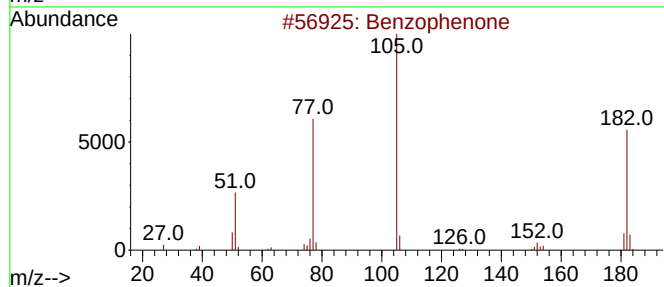
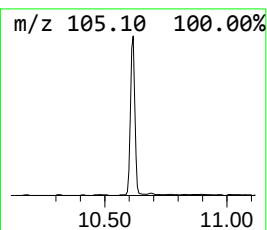
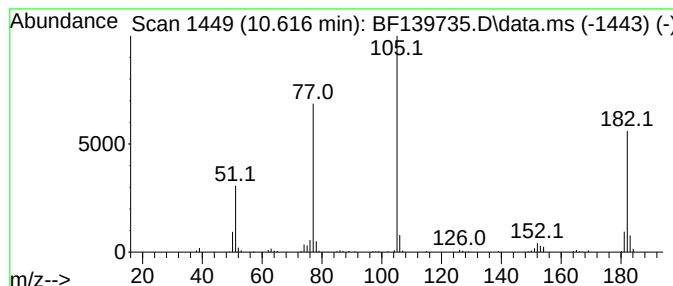
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.616	6.49 ng	192254	Acenaphthene-d10	9.904

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	53
3			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47
4			Methyl 2-benzoyl-4-cyanobutanoate	231	C13H13NO3	1010486-83-8	47
5			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47



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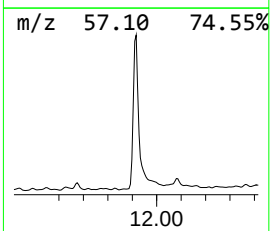
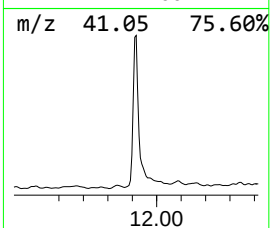
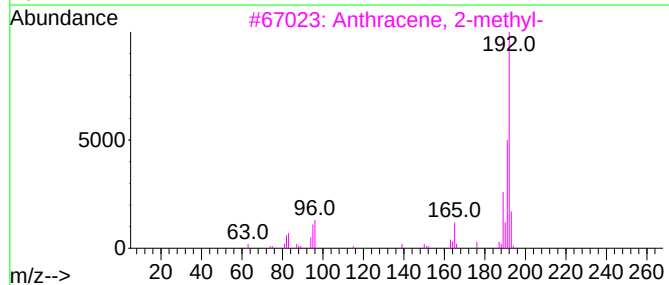
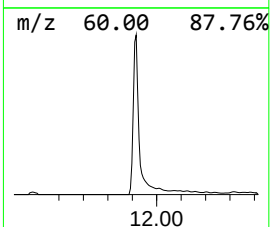
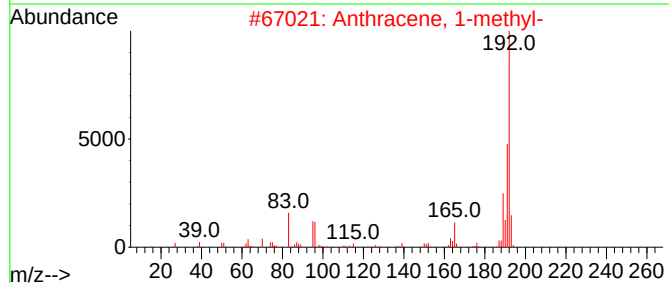
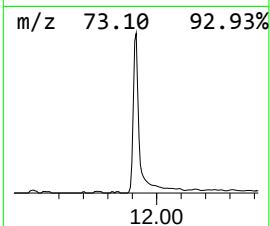
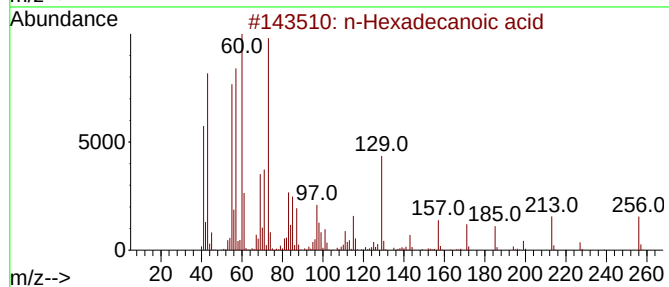
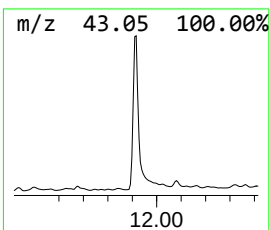
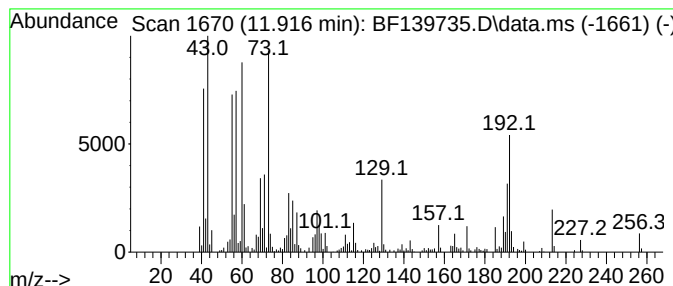
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	15.12 ng	445890	Phenanthrene-d10	11.386

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		Anthracene, 2-methyl-	192	C15H12	000613-12-7	86
4		Tridecanoic acid	214	C13H26O2	000638-53-9	78
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	64



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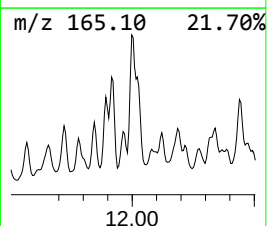
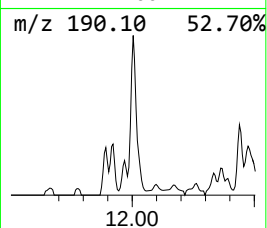
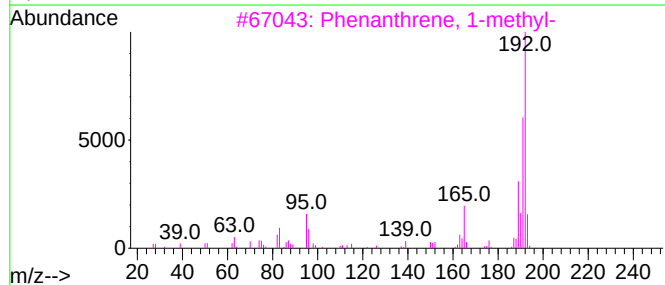
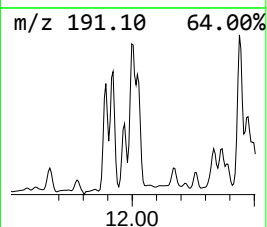
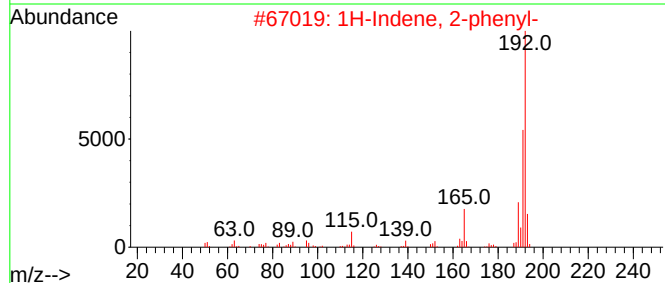
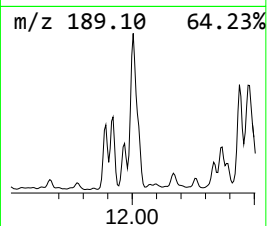
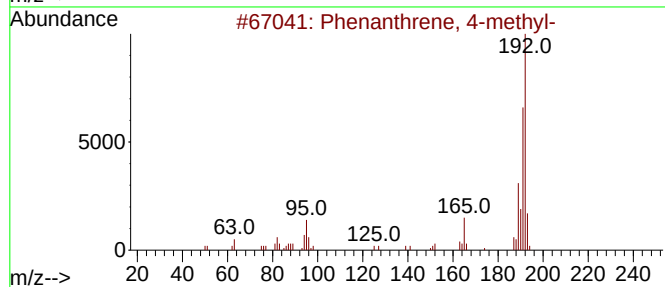
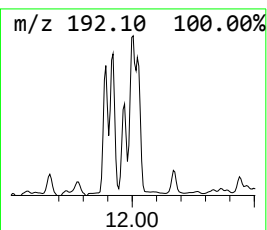
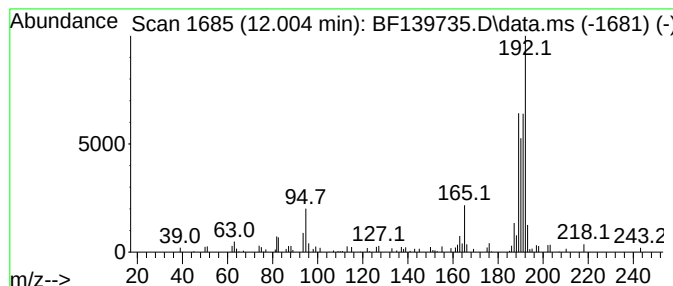
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Phenanthrene, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.004	4.80 ng	141712	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	60
2			1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	60
3			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	60
4			Anthracene, 1-methyl-	192	C15H12	000610-48-0	55
5			Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100924\
Data File : BF139735.D
Acq On : 09 Oct 2024 21:21
Operator : RC/JU
Sample : P4353-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CF-400-COMP-43

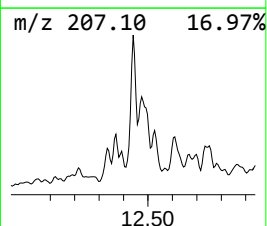
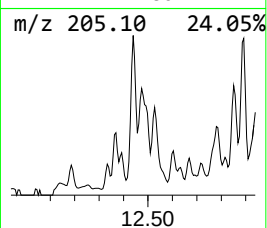
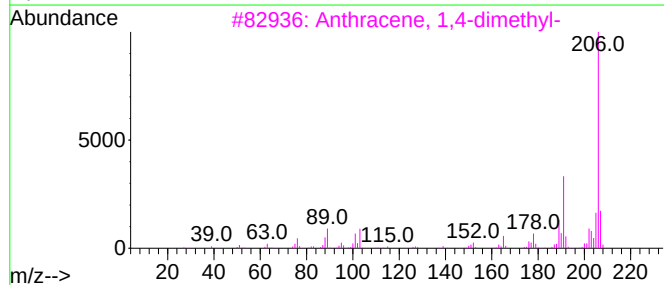
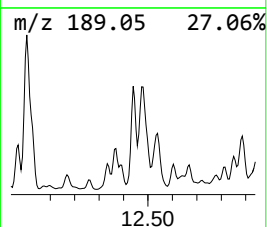
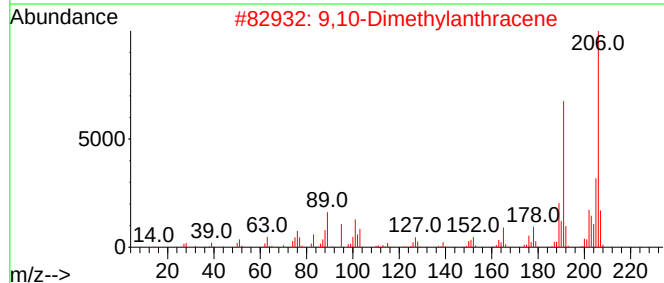
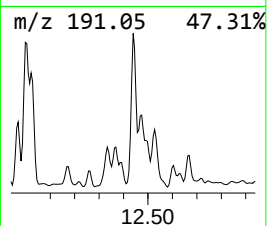
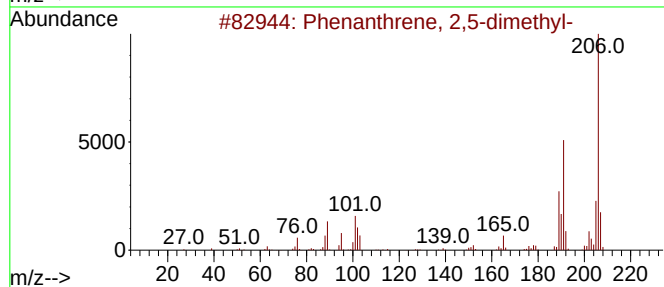
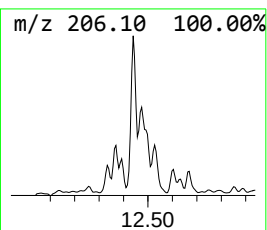
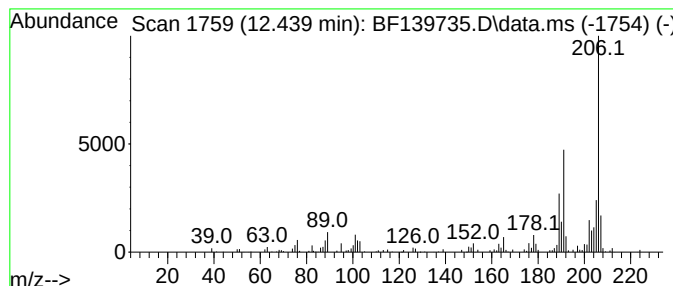
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Phenanthrene, 2,5-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.439	3.66 ng	107929	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	97
2			9,10-Dimethylantracene	206	C16H14	000781-43-1	95
3			Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	93
4			3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	91
5			Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100924\
Data File : BF139735.D
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ClientSampleId :
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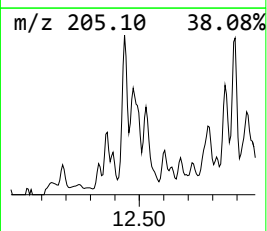
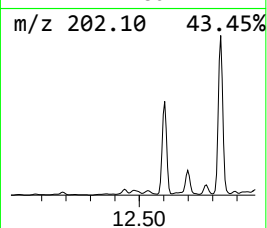
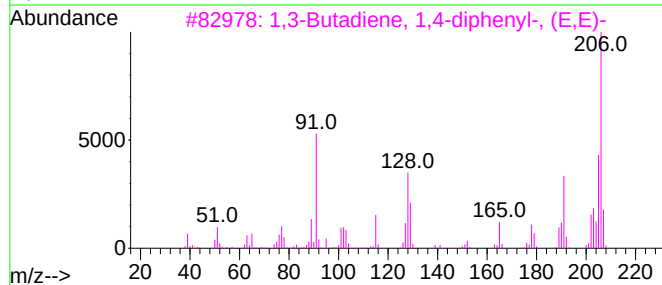
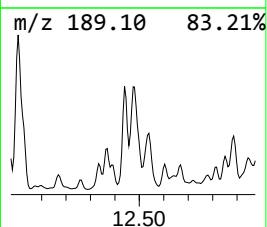
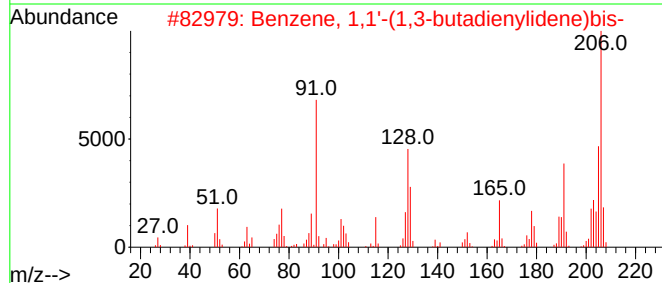
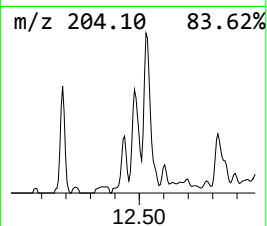
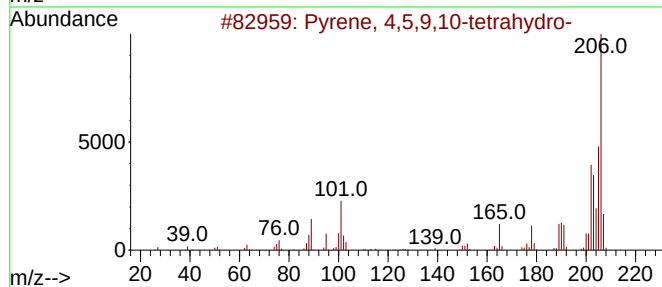
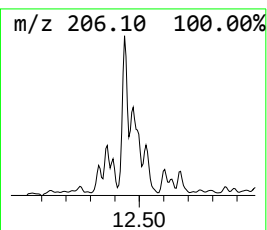
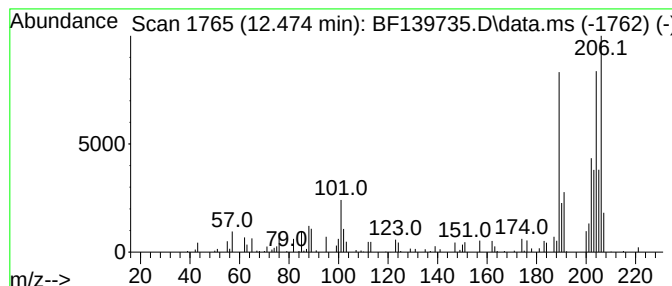
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown12.475 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.475	2.82 ng	83025	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene, 4,5,9,10-tetrahydro-	206	C16H14	000781-17-9	42
2			Benzene, 1,1'-(1,3-butadienylidene...	206	C16H14	004165-81-5	38
3			1,3-Butadiene, 1,4-diphenyl-, (E...	206	C16H14	000538-81-8	30
4			Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	30
5			Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100924\
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Operator : RC/JU
Sample : P4353-01
Misc :
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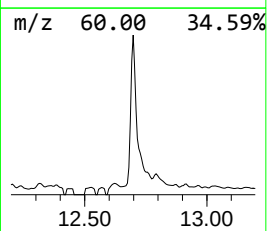
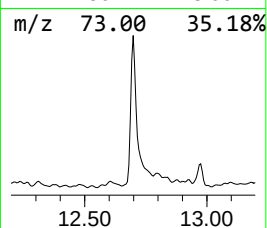
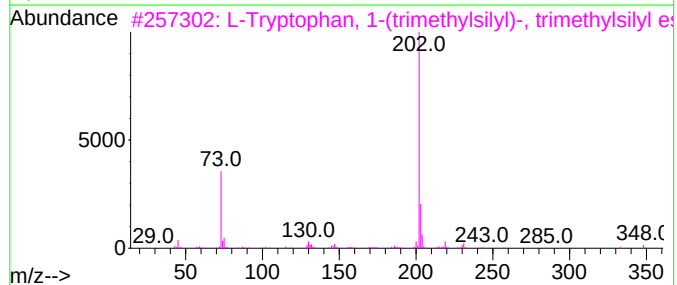
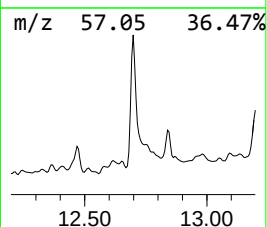
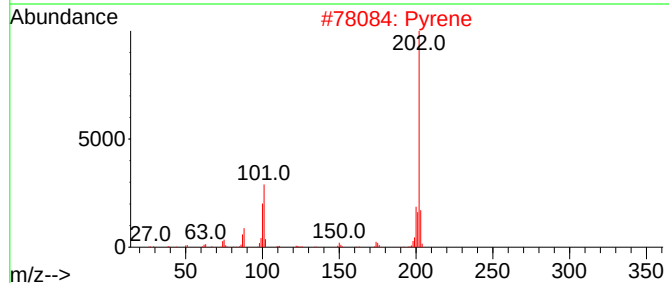
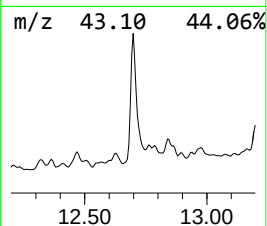
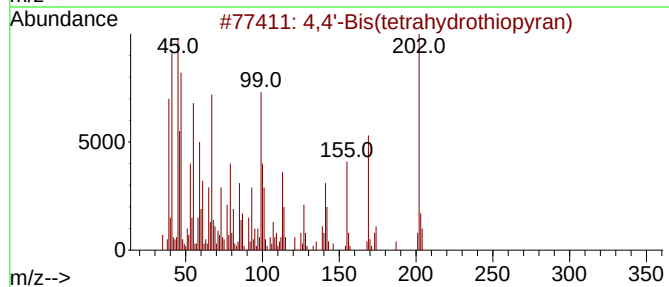
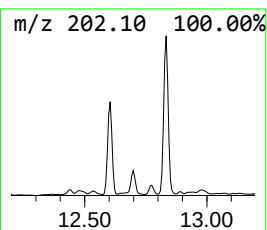
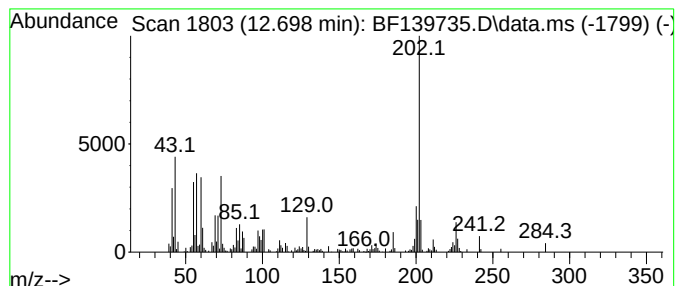
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 4,4'-Bis(tetrahydrothiopyran) Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.698	3.46 ng	102009	Phenanthrene-d10	11.386	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Bis(tetrahydrothiopyran)	202	C10H18S2	116196-83-9	93
2	Pyrene	202	C16H10	000129-00-0	50
3	L-Tryptophan, 1-(trimethylsilyl)...	348	C17H28N2O2Si2	1033331-59-7	47
4	L-Abrine, N-trimethylsilyl-, tri...	362	C18H30N2O2Si2	1000451-96-1	47
5	Fluoranthene	202	C16H10	000206-44-0	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100924\
Data File : BF139735.D
Acq On : 09 Oct 2024 21:21
Operator : RC/JU
Sample : P4353-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

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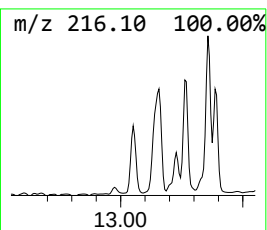
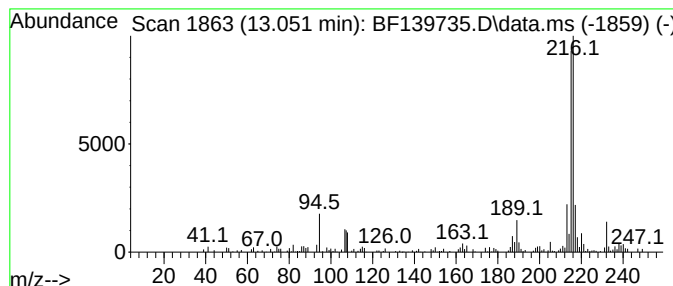
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 11H-Benzo[b]fluorene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.051	2.49 ng	100170	Chrysene-d12	14.033

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		11H-Benzo[b]fluorene	216	C17H12	000243-17-4	93
2		Pyrene, 1-methyl-	216	C17H12	002381-21-7	90
3		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	86
4		Pyrene, 2-methyl-	216	C17H12	003442-78-2	86
5		Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100924\
Data File : BF139735.D
Acq On : 09 Oct 2024 21:21
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Misc :
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Instrument :
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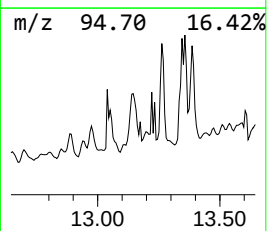
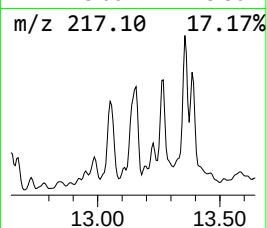
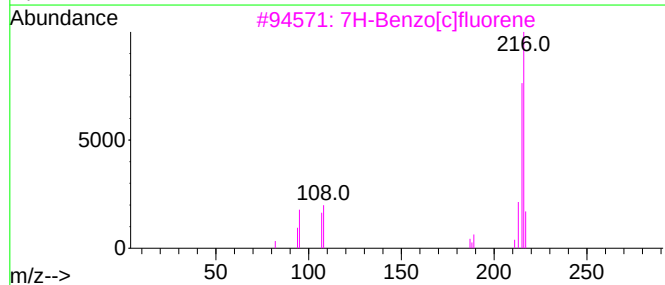
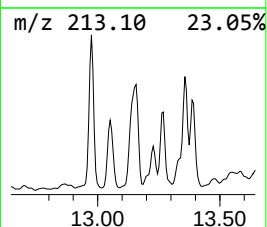
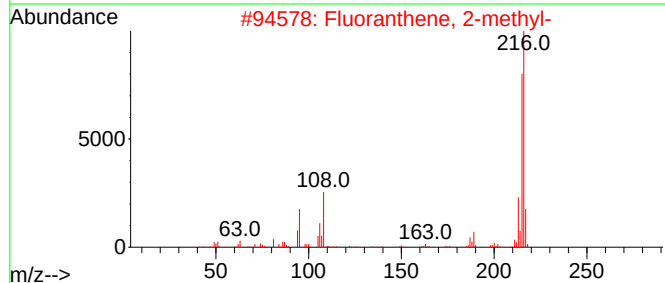
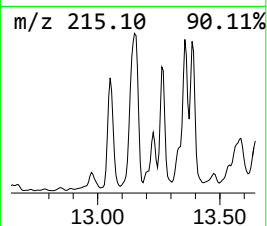
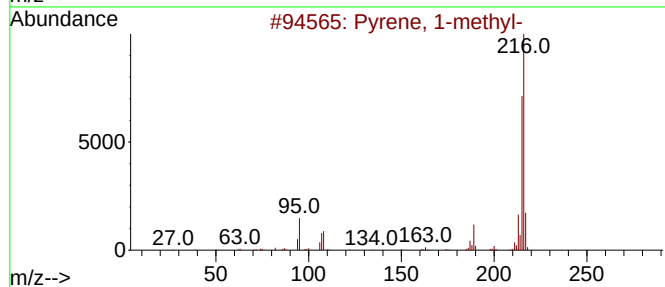
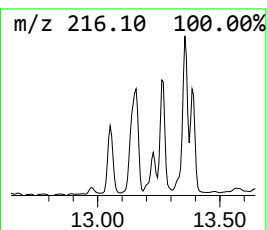
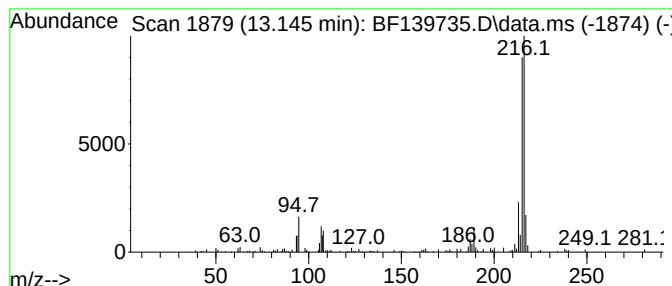
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Pyrene, 1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.145	3.36 ng	135479	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
2			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	90
3			7H-Benzo[c]fluorene	216	C17H12	000205-12-9	87
4			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	81
5			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100924\
Data File : BF139735.D
Acq On : 09 Oct 2024 21:21
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Misc :
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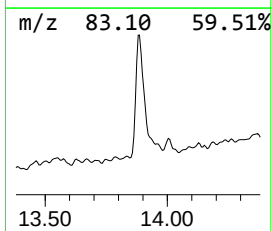
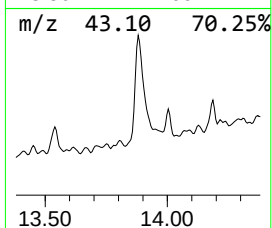
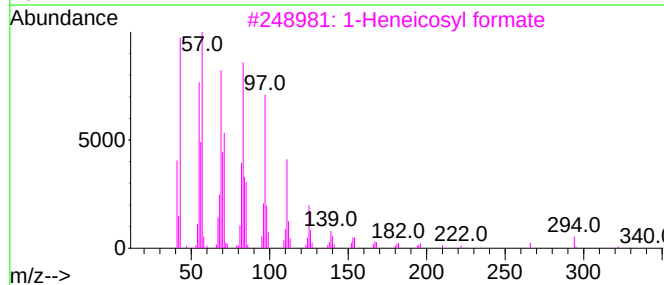
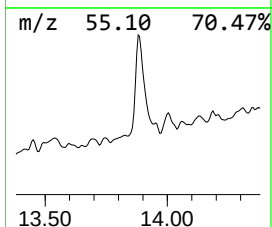
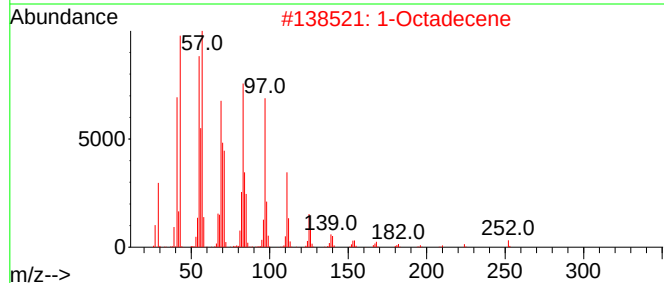
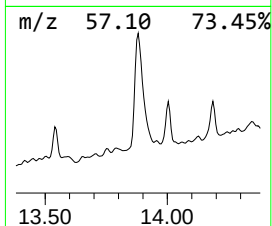
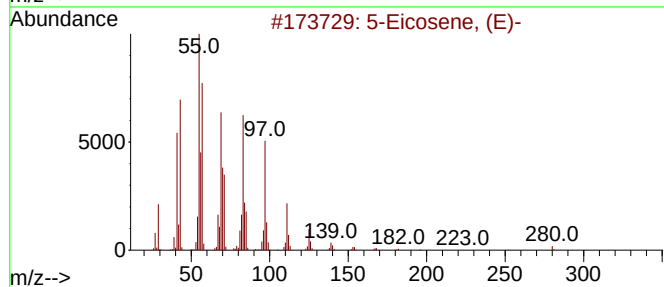
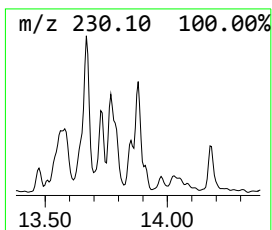
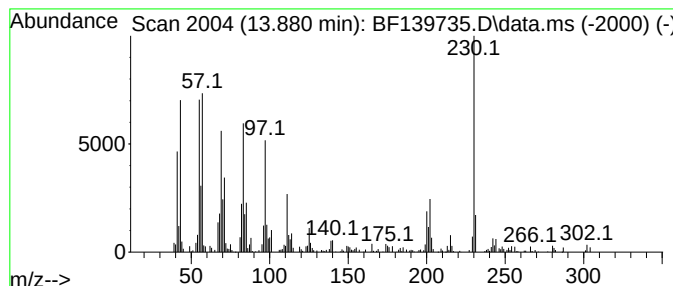
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 5-Eicosene, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	4.34 ng	174734	Chrysene-d12	14.033

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Eicosene, (E)-	280	C20H40	074685-30-6	93
2		1-Octadecene	252	C18H36	000112-88-9	93
3		1-Heneicosyl formate	340	C22H44O2	077899-03-7	84
4		Cycloeicosane	280	C20H40	000296-56-0	72
5		11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100924\
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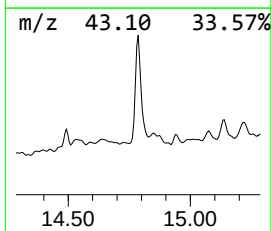
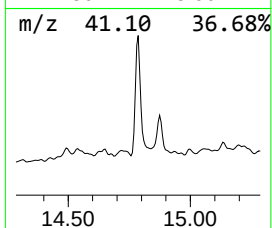
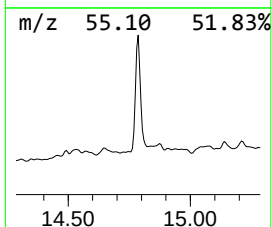
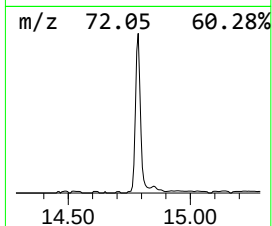
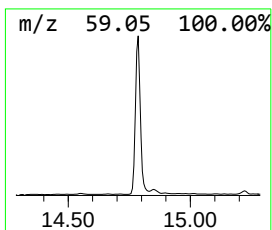
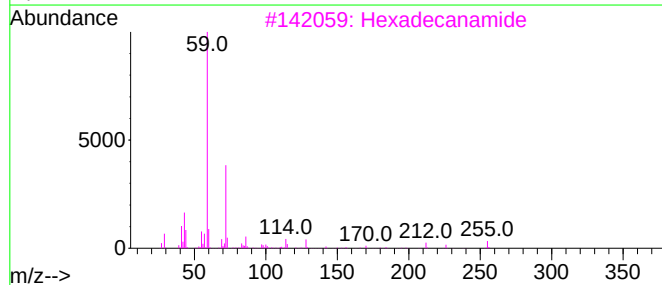
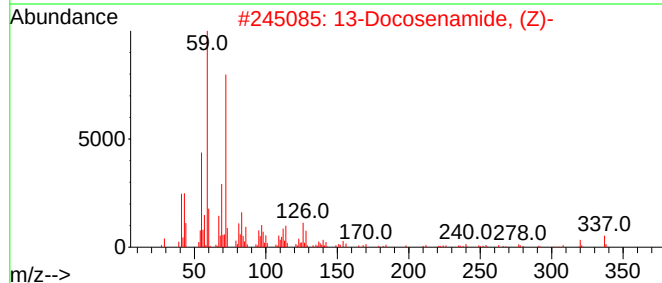
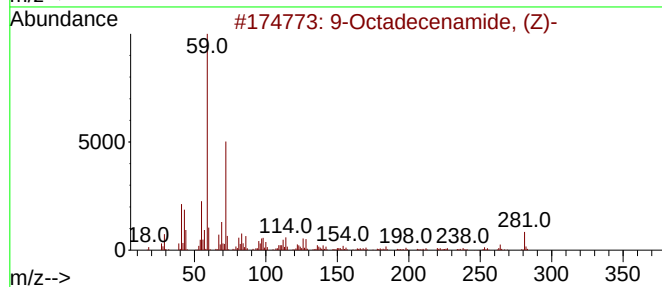
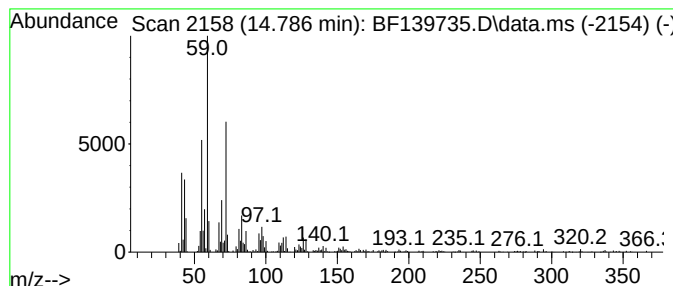
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.786	12.84 ng	244158	Perylene-d12	15.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	91
3			Hexadecanamide	255	C16H33NO	000629-54-9	78
4			9-Octadecenamide	281	C18H35NO	003322-62-1	78
5			Palmitoleamide	253	C16H31NO	106010-22-4	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100924\
Data File : BF139735.D
Acq On : 09 Oct 2024 21:21
Operator : RC/JU
Sample : P4353-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CF-400-COMP-43

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...	2.146	113.2	ng	2764950	1	6.869	488521	20.0
2-Pentanone, 4-...	5.081	5.3	ng	129102	1	6.869	488521	20.0
Benzophenone	10.616	6.5	ng	192254	3	9.904	592559	20.0
n-Hexadecanoic ...	11.916	15.1	ng	445890	4	11.386	589868	20.0
Phenanthrene, 4...	12.004	4.8	ng	141712	4	11.386	589868	20.0
Phenanthrene, 2...	12.439	3.7	ng	107929	4	11.386	589868	20.0
unknown12.475	12.475	2.8	ng	83025	4	11.386	589868	20.0
4,4'-Bis(tetra...	12.698	3.5	ng	102009	4	11.386	589868	20.0
11H-Benzo[b]flu...	13.051	2.5	ng	100170	5	14.033	805448	20.0
Pyrene, 1-methyl-	13.145	3.4	ng	135479	5	14.033	805448	20.0
5-Eicosene, (E)-	13.880	4.3	ng	174734	5	14.033	805448	20.0
9-Octadecenamid...	14.786	12.8	ng	244158	6	15.510	380454	20.0