

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
 Data File : BF139311.D
 Acq On : 10 Sep 2024 20:59
 Operator : RC/JU
 Sample : P3906-13 5X
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SU-701-COMP-03

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-BF090424.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139311.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	6	12	19	rVB	242803	380482	42.19%	3.538%
2	5.087	504	509	518	rVB	31730	42452	4.71%	0.395%
3	5.493	573	578	586	rBV	399095	501395	55.60%	4.662%
4	6.504	745	750	762	rBV	436288	535176	59.34%	4.976%
5	6.887	810	815	820	rBV	535693	642561	71.25%	5.974%
6	7.445	904	910	915	rBV	275308	344460	38.20%	3.203%
7	7.698	949	953	960	rVB	9473	11867	1.32%	0.110%
8	8.169	1028	1033	1040	rBV	664666	795499	88.21%	7.396%
9	9.239	1210	1215	1226	rBV	506084	632061	70.09%	5.877%
10	9.781	1303	1307	1312	rBV	11350	13979	1.55%	0.130%
11	9.922	1326	1331	1336	rBV	651853	803588	89.11%	7.471%
12	10.633	1447	1452	1459	rVB	48255	60295	6.69%	0.561%
13	10.704	1459	1464	1476	rVB	208946	276422	30.65%	2.570%
14	10.833	1481	1486	1490	rBV2	7757	10389	1.15%	0.097%
15	11.351	1571	1574	1577	rBV3	7526	10428	1.16%	0.097%
16	11.410	1578	1584	1592	rVV2	531807	775429	85.98%	7.210%
17	11.480	1592	1596	1600	rVB	12744	17286	1.92%	0.161%
18	11.639	1617	1623	1628	rBV2	9864	17684	1.96%	0.164%
19	11.863	1657	1661	1664	rBV4	6222	9122	1.01%	0.085%
20	11.933	1664	1673	1678	rBV2	82480	150000	16.63%	1.395%
21	12.022	1684	1688	1696	rVB2	36155	71616	7.94%	0.666%
22	12.110	1698	1703	1706	rBV6	10205	17212	1.91%	0.160%
23	12.227	1716	1723	1728	rVB3	18088	40846	4.53%	0.380%
24	12.351	1738	1744	1747	rBV6	8075	12710	1.41%	0.118%
25	12.457	1758	1762	1765	rBV	26478	35675	3.96%	0.332%
26	12.498	1765	1769	1774	rVV3	15246	28877	3.20%	0.268%
27	12.545	1774	1777	1782	rVB3	20383	28217	3.13%	0.262%
28	12.622	1785	1790	1794	rBV	243167	309678	34.34%	2.879%
29	12.716	1803	1806	1809	rBV2	12664	12903	1.43%	0.120%
30	12.851	1821	1829	1835	rBV	228850	355644	39.44%	3.307%
31	12.898	1835	1837	1840	rVV3	9378	11267	1.25%	0.105%
32	12.933	1840	1843	1846	rVV	32324	35735	3.96%	0.332%
33	12.992	1848	1853	1859	rVB	352883	453378	50.27%	4.215%
34	13.057	1859	1864	1870	rBV5	29976	65097	7.22%	0.605%
35	13.174	1877	1884	1888	rVB2	28719	57504	6.38%	0.535%
36	13.239	1888	1895	1898	rBV3	21807	52995	5.88%	0.493%

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Peak Location: TOP

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37	13.280	1898	1902	1906	rVV3	27703	40643	4.51%	0.378%
38	13.374	1915	1918	1920	rBV	16663	18106	2.01%	0.168%
39	13.404	1920	1923	1927	rVV	18675	21406	2.37%	0.199%
40	13.469	1930	1934	1941	rVB	60687	81550	9.04%	0.758%
41	13.680	1967	1970	1975	rVB	29829	42800	4.75%	0.398%
42	13.792	1985	1989	1992	rBV2	24940	42892	4.76%	0.399%
43	13.892	2002	2006	2016	rVB3	69740	114488	12.69%	1.064%
44	14.045	2025	2032	2045	rBV2	487611	901839	100.00%	8.385%
45	14.527	2109	2114	2127	rVB6	72346	224811	24.93%	2.090%
46	14.974	2186	2190	2198	rBV2	70308	108015	11.98%	1.004%
47	15.092	2205	2210	2220	rVB	118295	279810	31.03%	2.602%
48	15.174	2220	2224	2225	rBV3	32985	43150	4.78%	0.401%
49	15.198	2225	2228	2241	rVB3	74826	163266	18.10%	1.518%
50	15.392	2257	2261	2267	rVB	57521	87509	9.70%	0.814%
51	15.457	2267	2272	2277	rVB	75483	116957	12.97%	1.087%
52	15.521	2278	2283	2295	rVB	245158	427402	47.39%	3.974%
53	16.004	2361	2365	2370	rBV	45139	71323	7.91%	0.663%
54	16.992	2530	2533	2546	rVB2	38976	91902	10.19%	0.854%
55	17.609	2631	2638	2647	rBV7	45961	158091	17.53%	1.470%
56	17.851	2674	2679	2694	rVB7	37040	99669	11.05%	0.927%

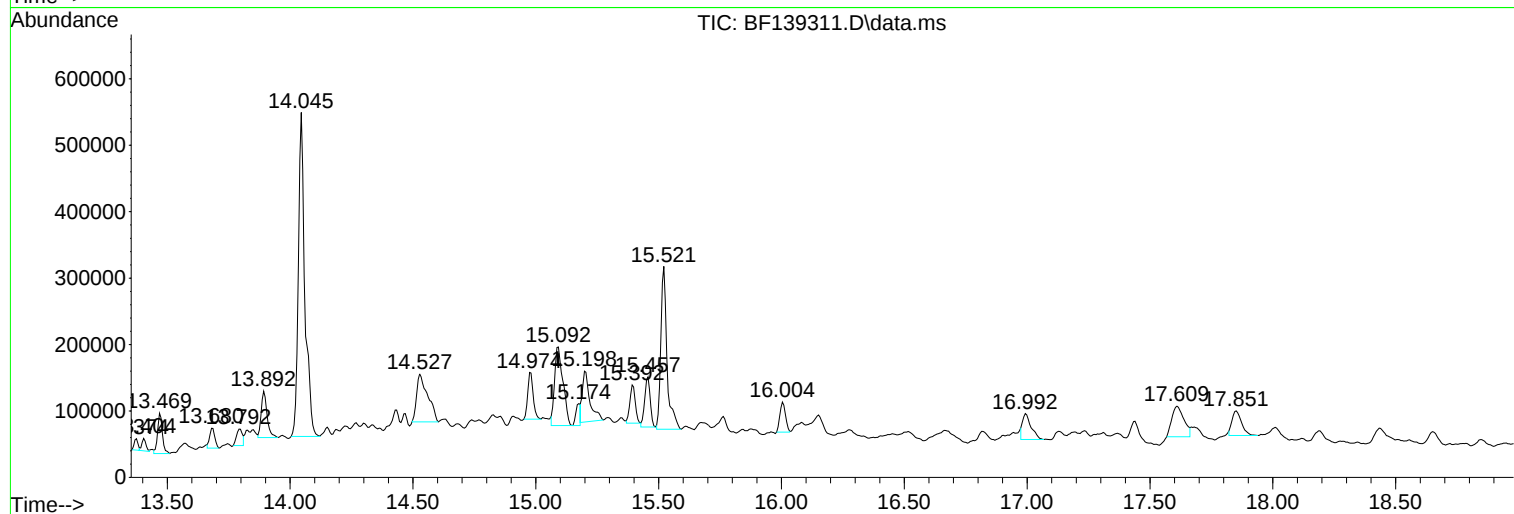
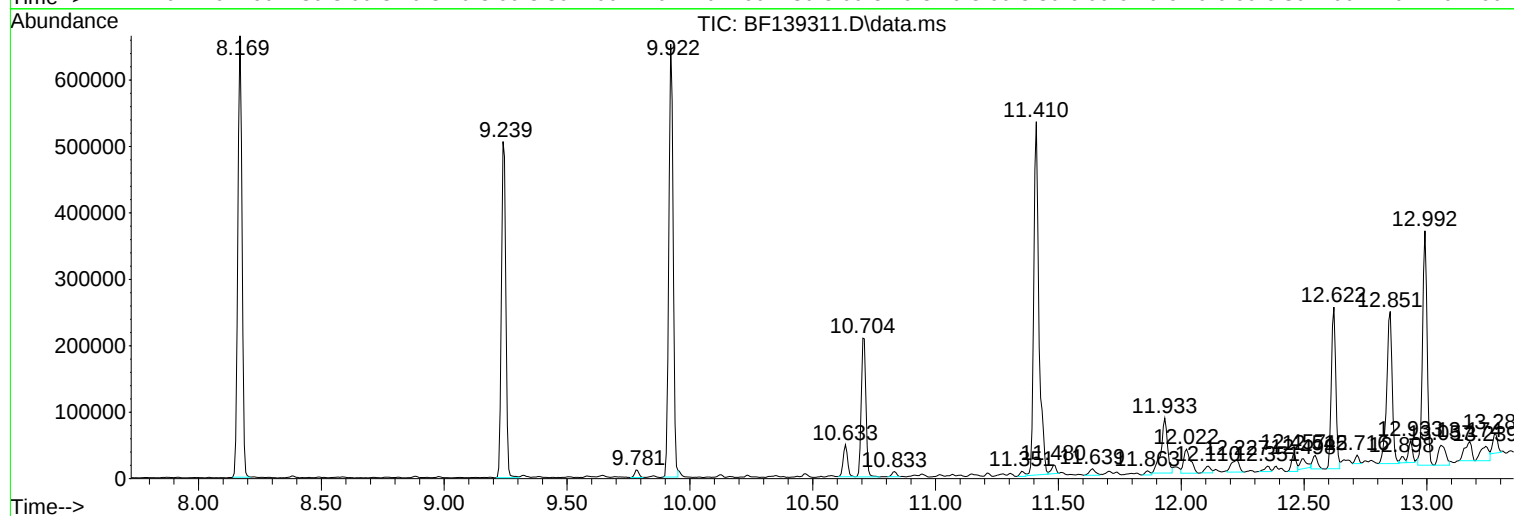
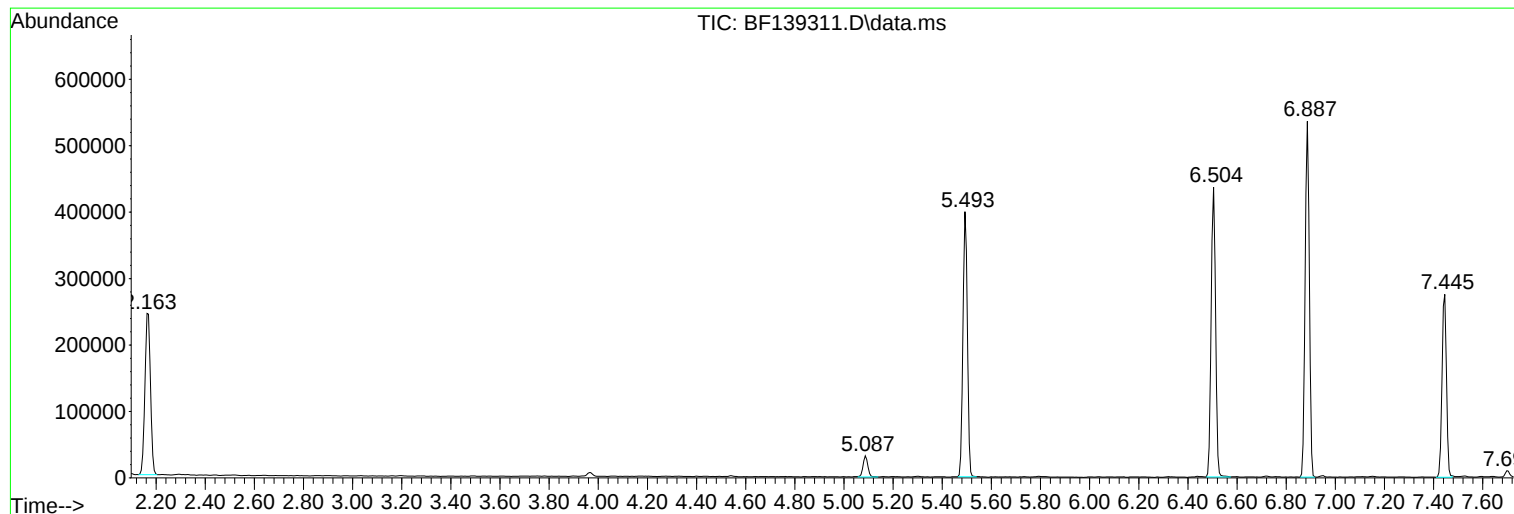
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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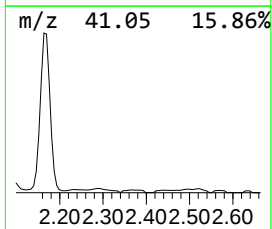
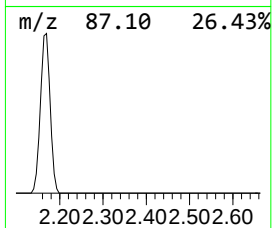
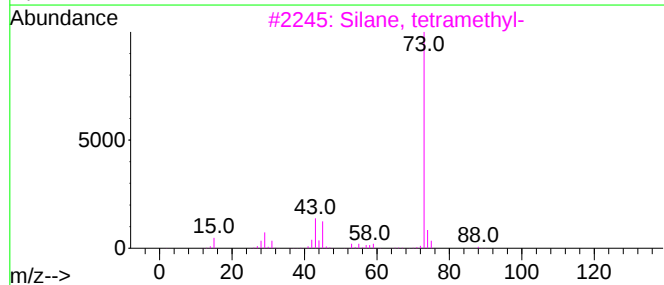
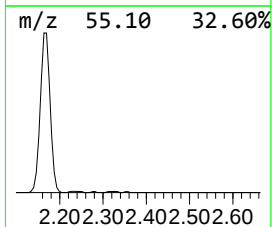
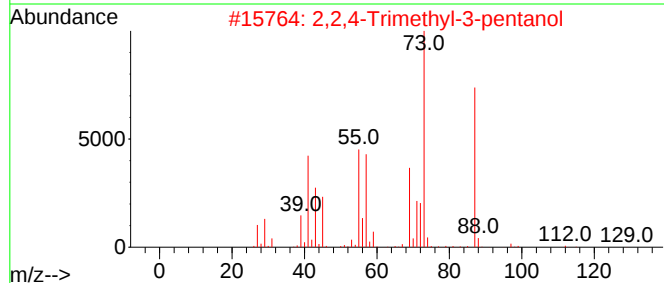
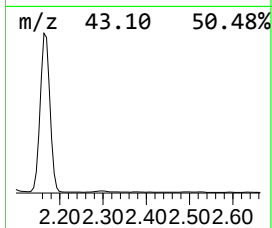
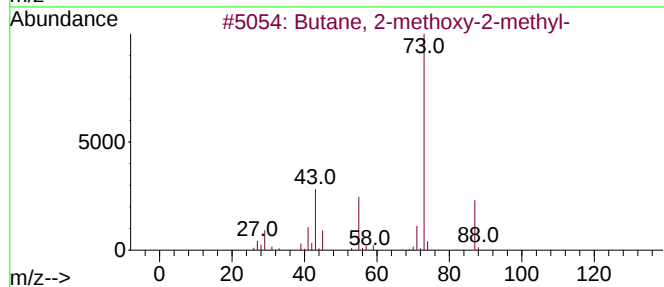
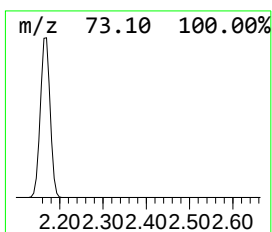
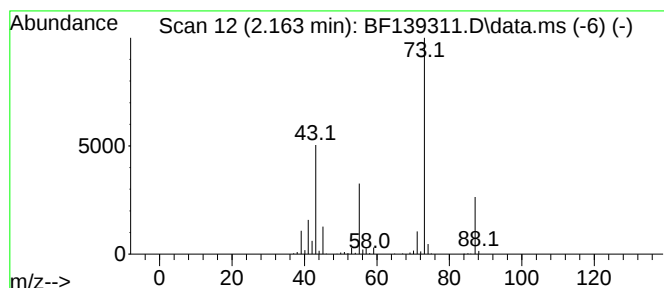
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	11.84 ng	380482	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			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	38
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32



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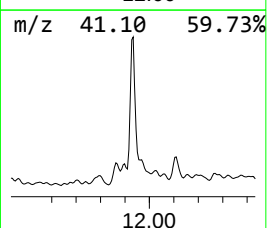
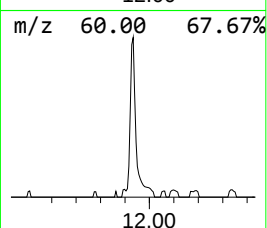
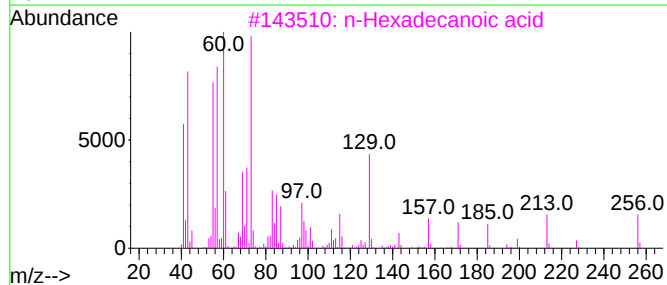
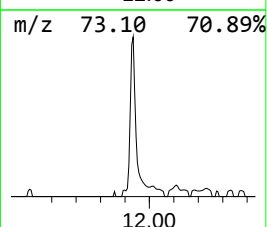
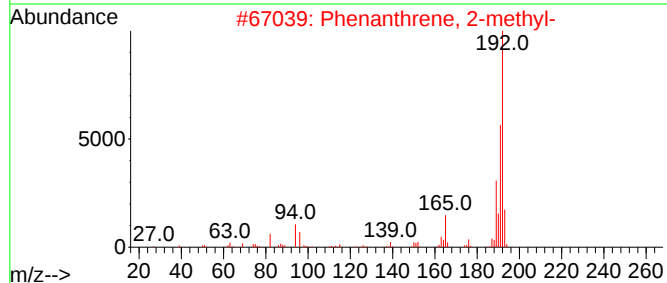
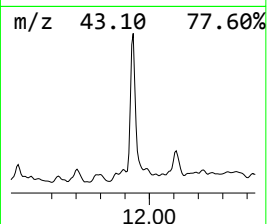
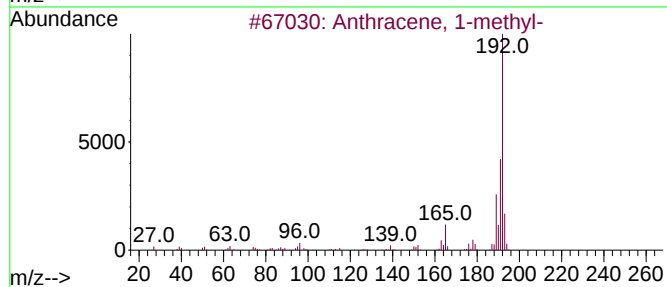
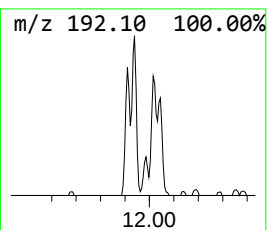
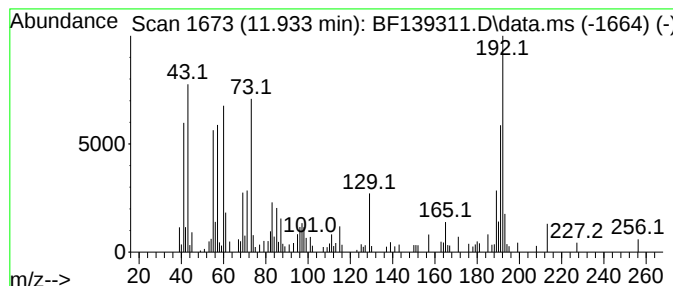
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Anthracene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	3.87 ng	150000	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 1-methyl-	192	C15H12	000610-48-0	95
2			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
4			Anthracene, 2-methyl-	192	C15H12	000613-12-7	92
5			Anthracene, 9-methyl-	192	C15H12	000779-02-2	91



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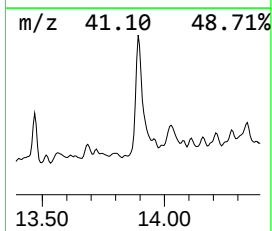
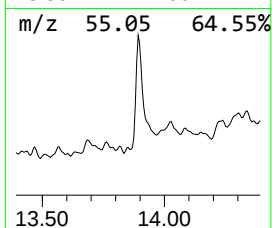
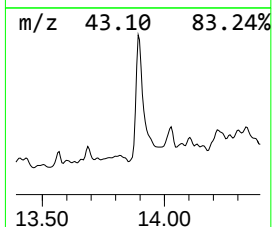
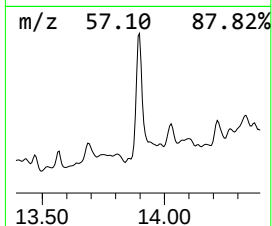
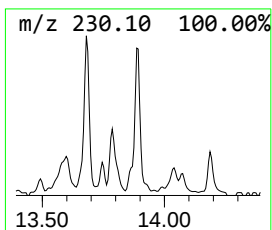
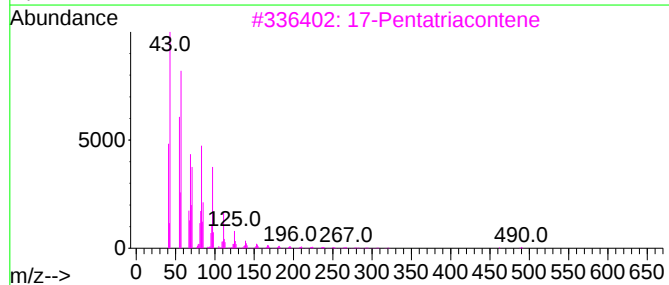
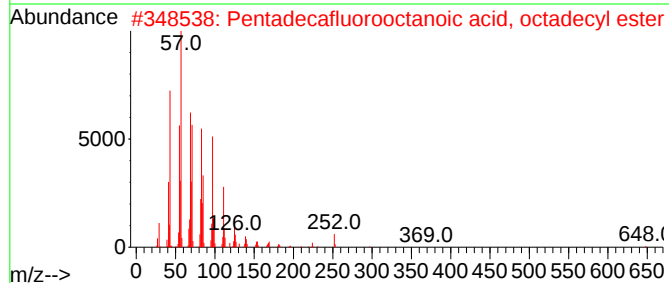
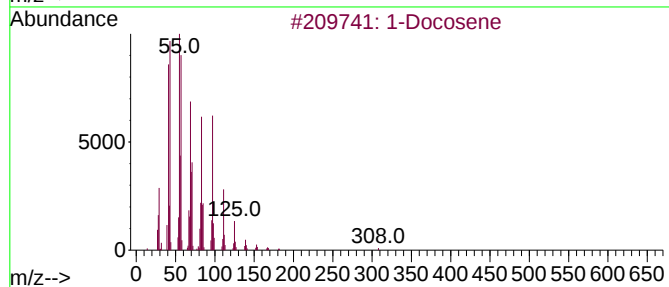
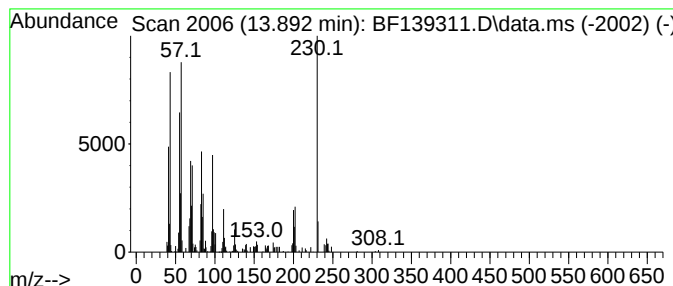
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Docosene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	2.54 ng	114488	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Docosene	308	C22H44	001599-67-3	96
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	70
3			17-Pentatriacontene	491	C35H70	006971-40-0	55
4			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	55
5			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	55



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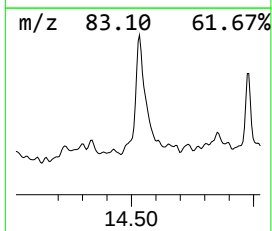
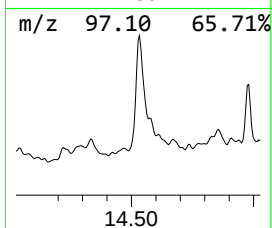
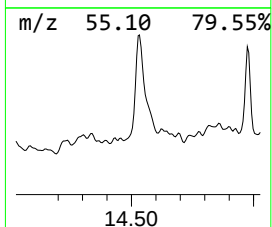
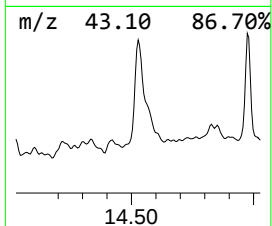
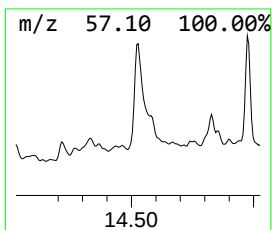
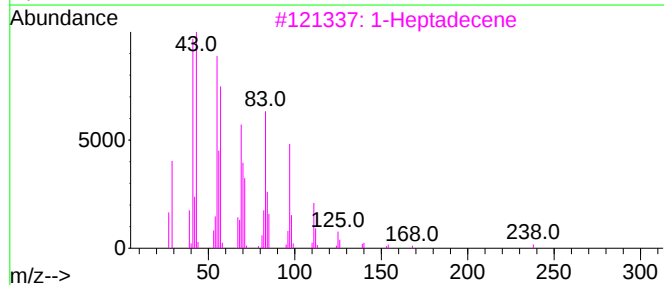
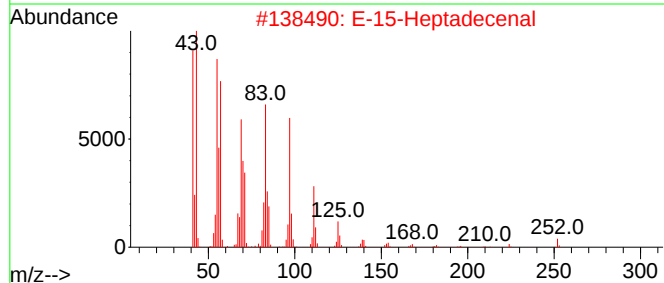
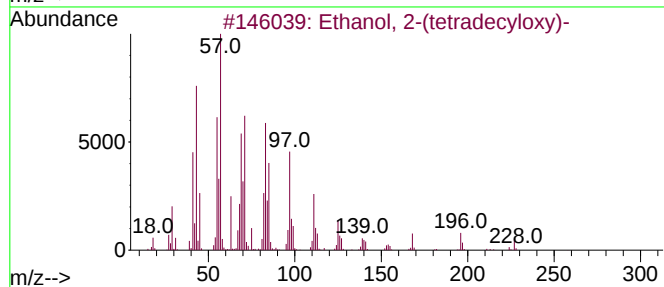
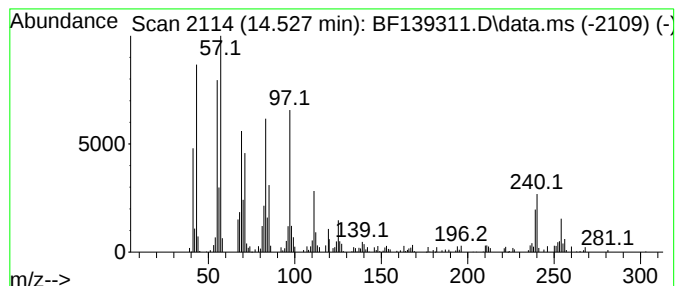
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Ethanol, 2-(tetradecyloxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.527	4.99 ng	224811	Chrysene-d12		14.045	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-		258	C16H34O2	002136-70-1	86
2	E-15-Heptadecenal		252	C17H32O	1000130-97-9	86
3	1-Heptadecene		238	C17H34	006765-39-5	83
4	Heptafluorobutyric acid, n-octad...		466	C22H37F7O2	000400-57-7	70
5	Tricosyl trifluoroacetate		436	C25H47F3O2	1000351-75-1	70



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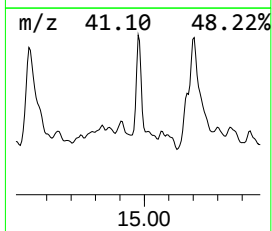
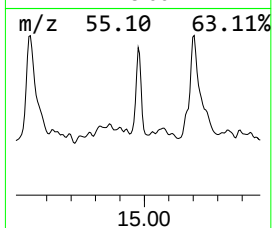
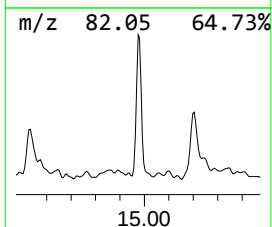
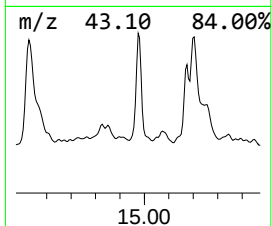
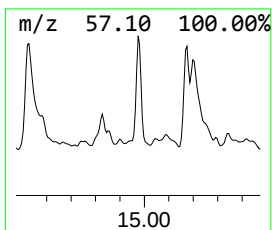
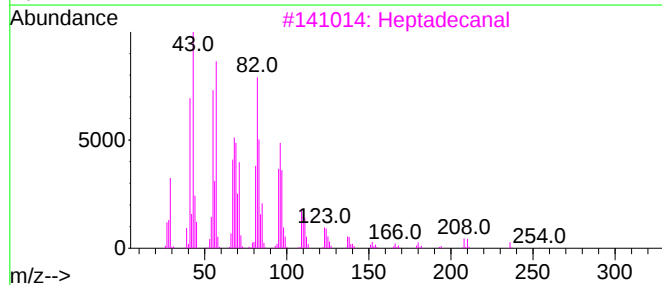
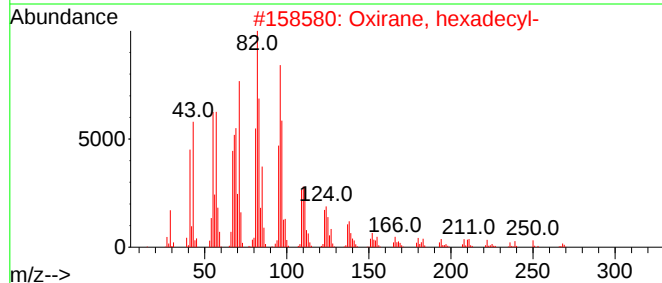
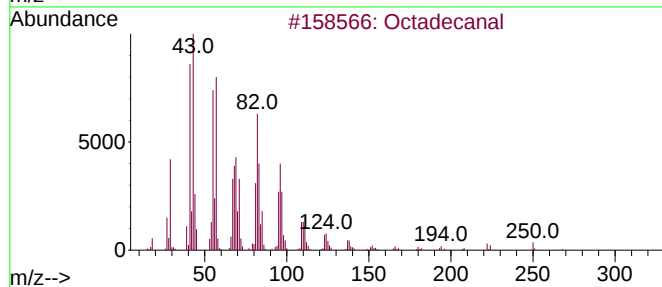
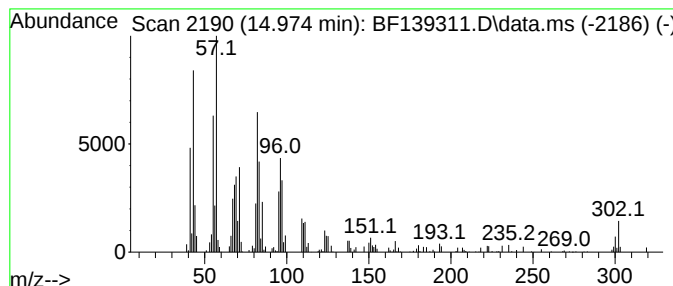
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.974	5.05 ng	108015	Perylene-d12	15.521

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanal	268	C18H36O	000638-66-4	93
2			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87
3			Heptadecanal	254	C17H34O	1000376-70-0	72
4			1,19-Eicosadiene	278	C20H38	014811-95-1	70
5			Eicosanal-	296	C20H40O	002400-66-0	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139311.D
Acq On : 10 Sep 2024 20:59
Operator : RC/JU
Sample : P3906-13 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-701-COMP-03

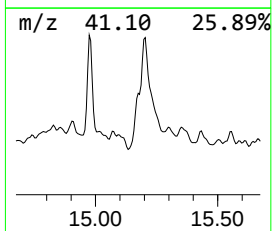
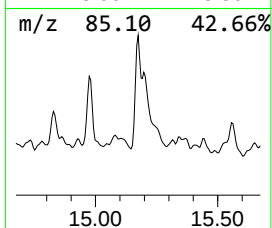
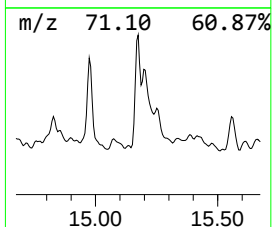
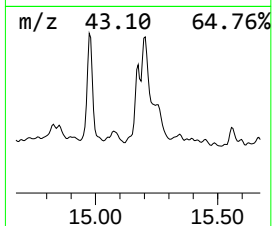
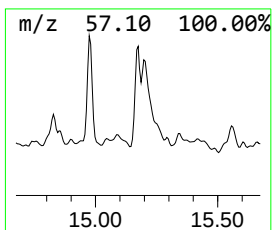
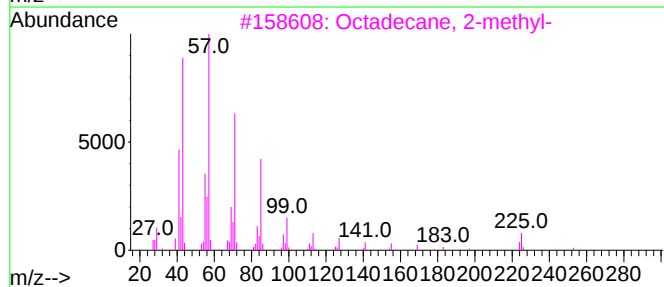
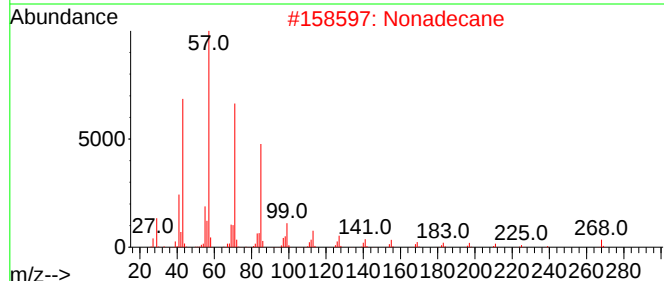
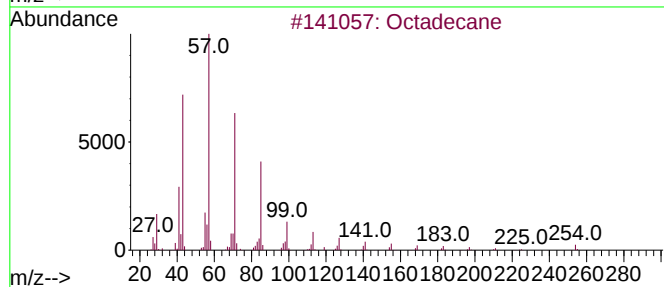
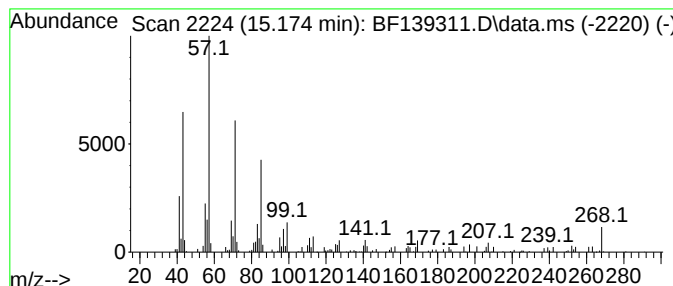
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.174	2.02 ng	43150	Perylene-d12	15.521

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	95
2			Nonadecane	268	C19H40	000629-92-5	90
3			Octadecane, 2-methyl-	268	C19H40	001560-88-9	80
4			Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1010309-18-1	80
5			Heptacosane	380	C27H56	000593-49-7	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139311.D
Acq On : 10 Sep 2024 20:59
Operator : RC/JU
Sample : P3906-13 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-701-COMP-03

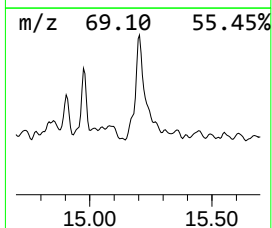
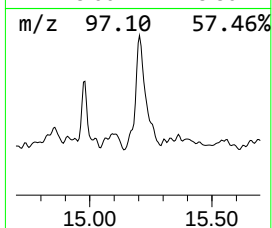
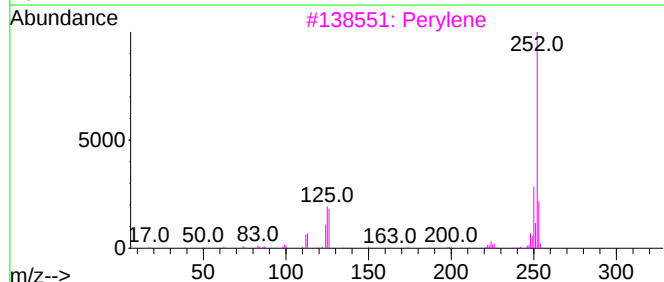
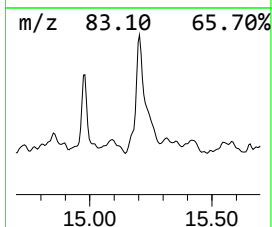
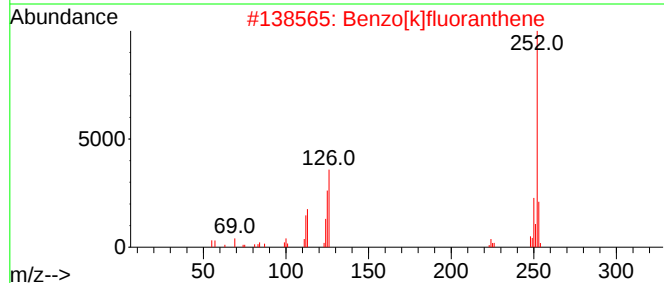
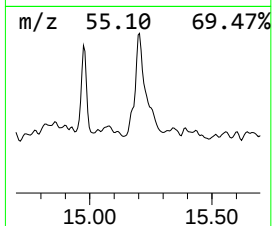
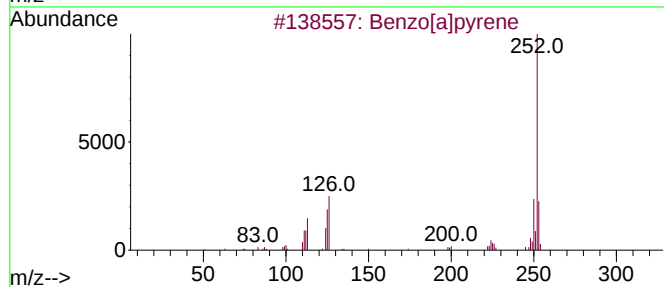
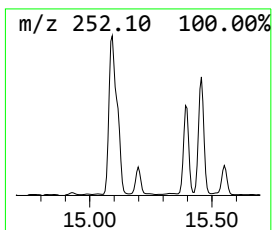
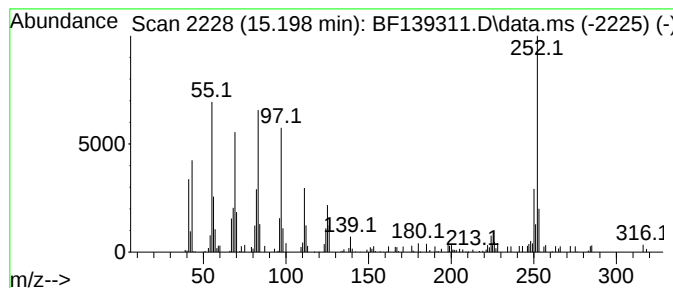
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown15.198 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.198	7.64 ng	163266	Perylene-d12	15.521

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[a]pyrene	252	C20H12	000050-32-8	64
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	55
3			Perylene	252	C20H12	000198-55-0	45
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	43
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	41



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139311.D
Acq On : 10 Sep 2024 20:59
Operator : RC/JU
Sample : P3906-13 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-701-COMP-03

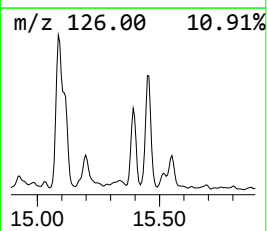
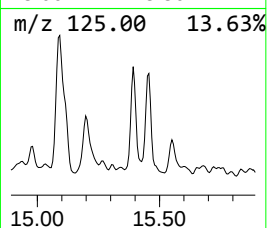
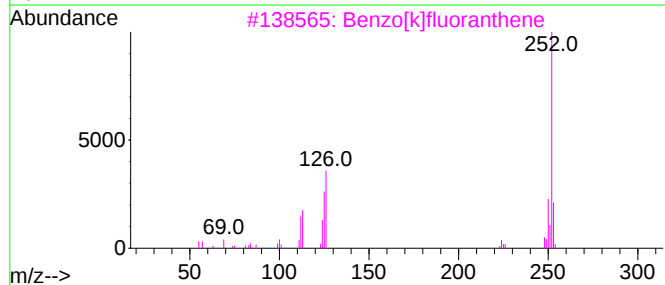
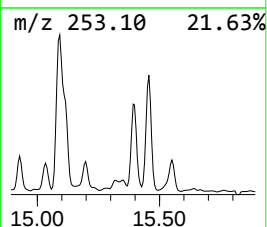
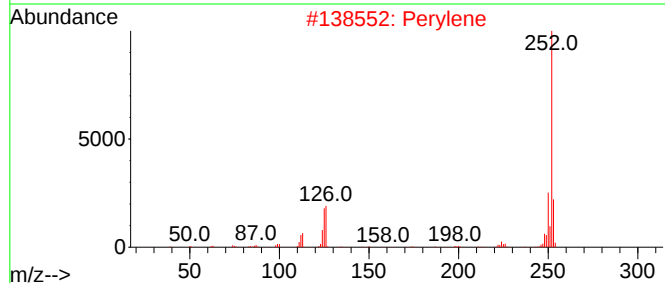
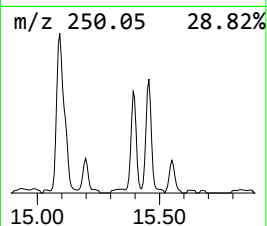
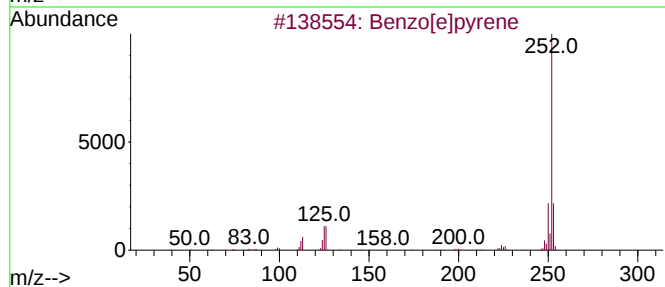
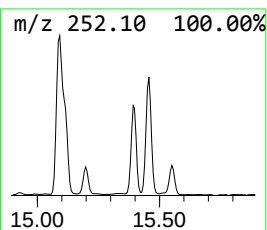
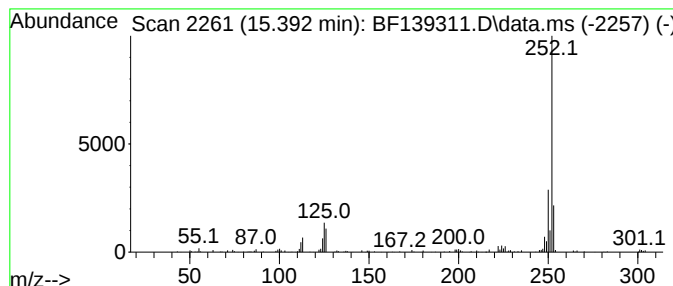
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.392	4.09 ng	87509	Perylene-d12	15.521

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	94
2			Perylene	252	C20H12	000198-55-0	93
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	91
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	91
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139311.D
Acq On : 10 Sep 2024 20:59
Operator : RC/JU
Sample : P3906-13 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-701-COMP-03

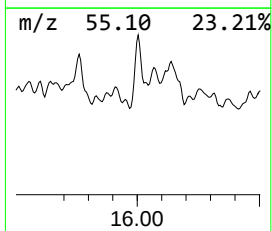
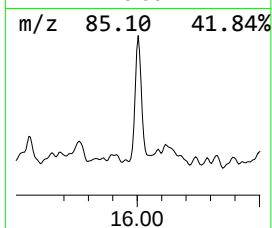
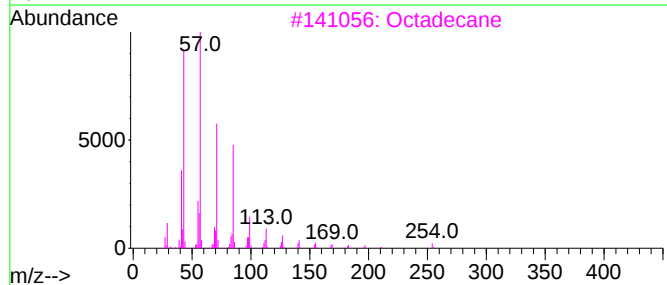
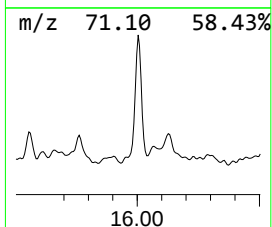
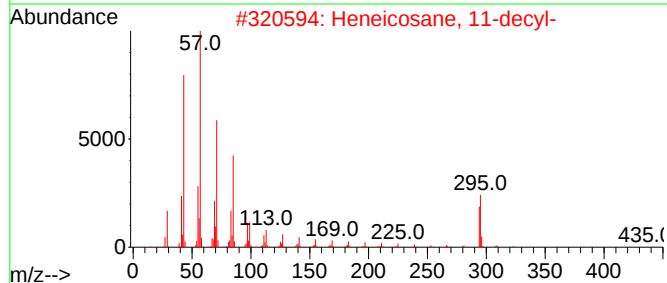
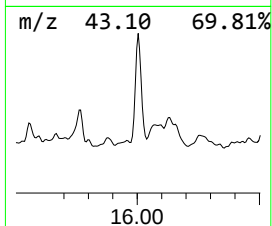
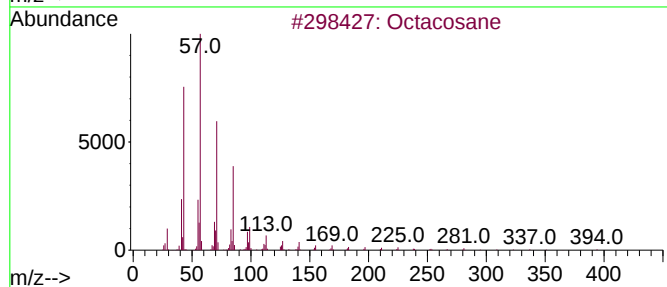
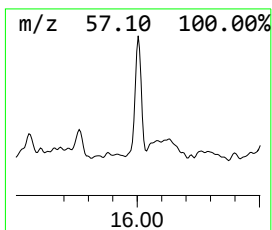
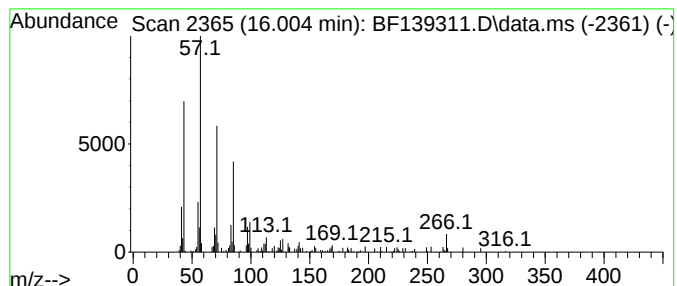
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.004	3.34 ng	71323	Perylene-d12	15.521

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	87
2			Heneicosane, 11-decyl-	437	C31H64	055320-06-4	87
3			Octadecane	254	C18H38	000593-45-3	83
4			Hentriacontane	437	C31H64	000630-04-6	83
5			Tetracosane	338	C24H50	000646-31-1	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139311.D
Acq On : 10 Sep 2024 20:59
Operator : RC/JU
Sample : P3906-13 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-701-COMP-03

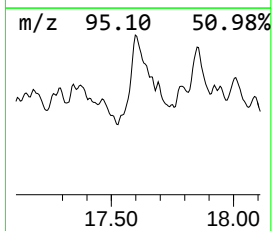
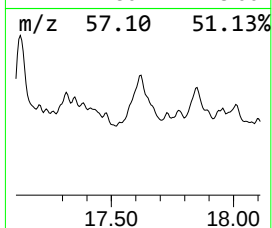
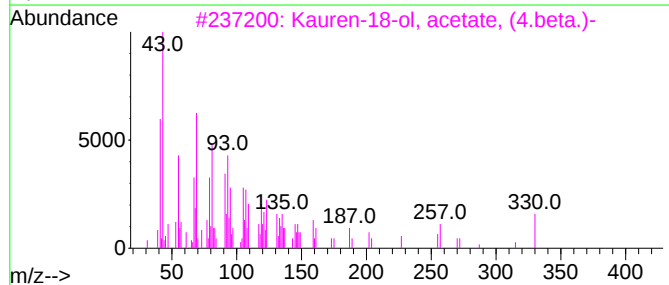
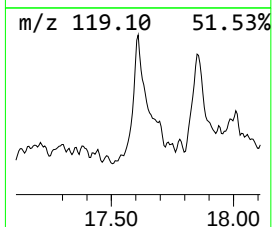
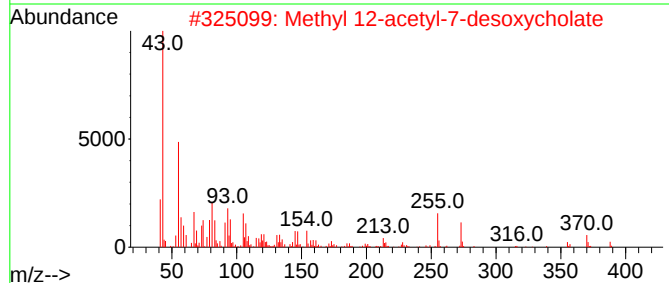
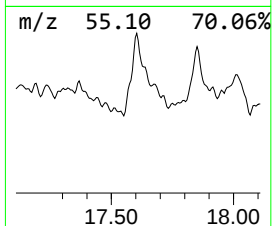
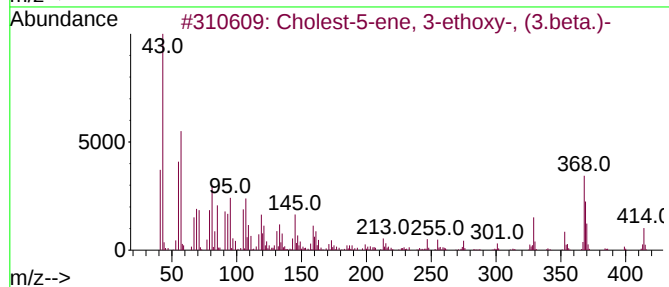
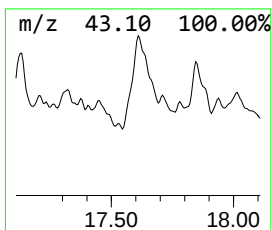
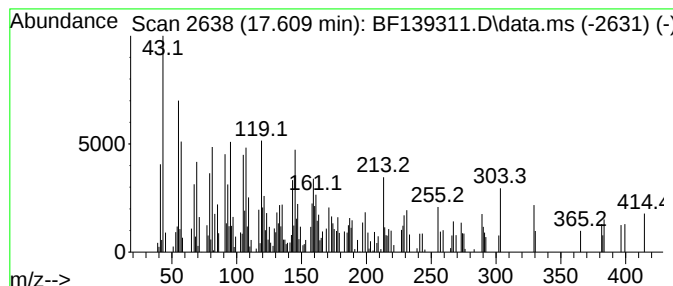
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Cholest-5-ene, 3-ethoxy-, (... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.609	7.40 ng	158091	Perylene-d12	15.521

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	55
2			Methyl 12-acetyl-7-desoxycholate	448	C27H44O5	055547-48-3	37
3			Kauren-18-ol, acetate, (4.beta.)-	330	C22H34O2	072150-74-4	25
4			Benzoic acid, 2-[(4H-pyrazole-3-...	231	C11H9N3O3	1000303-61-9	18
5			.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	16



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139311.D
Acq On : 10 Sep 2024 20:59
Operator : RC/JU
Sample : P3906-13 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-701-COMP-03

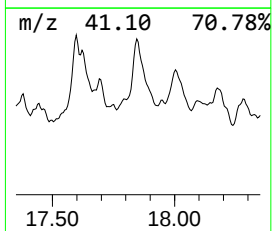
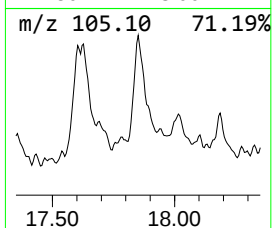
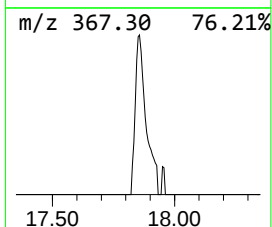
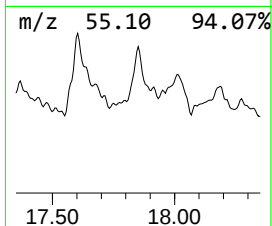
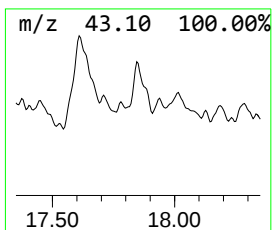
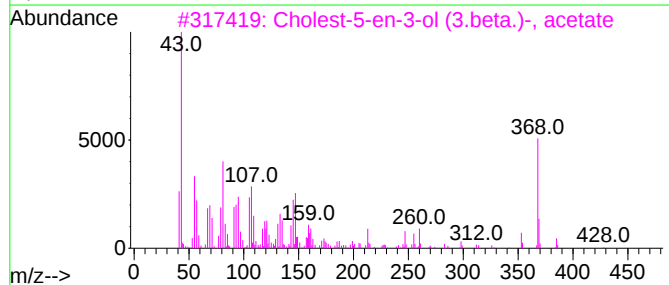
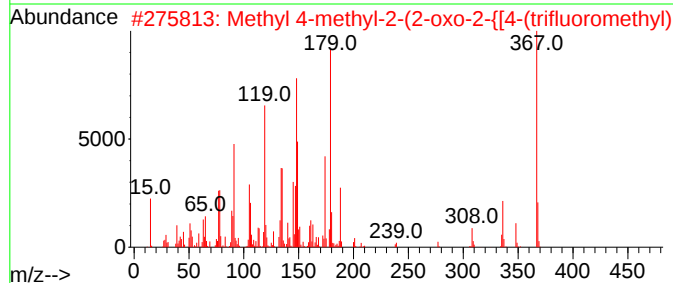
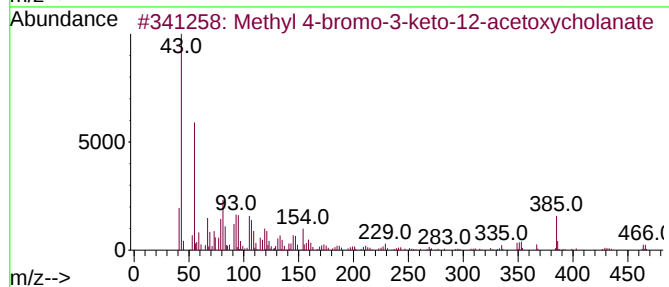
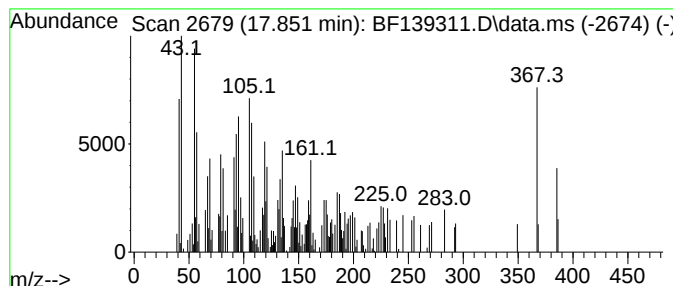
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown17.851 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.851	4.66 ng	99669	Perylene-d12	15.521

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl 4-bromo-3-keto-12-acetoxy...	524	C27H41BrO5	1000251-88-4	41
2			Methyl 4-methyl-2-(2-oxo-2-{[4-(...	367	C18H16F3NO4	1000460-31-9	35
3			Cholest-5-en-3-ol (3.beta.)-, ac...	428	C29H48O2	000604-35-3	30
4			7.beta.,17.alpha.-Dimethyl-5.bet...	320	C21H36O2	153546-23-7	25
5			1H-2,8a-Methanocyclopenta[a]cycl...	474	C26H34O8	030220-45-2	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139311.D
Acq On : 10 Sep 2024 20:59
Operator : RC/JU
Sample : P3906-13 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-701-COMP-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.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...	2.163	11.8	ng	380482	1	6.887	642561	20.0
Anthracene, 1-m...	11.933	3.9	ng	150000	4	11.410	775429	20.0
1-Docosene	13.892	2.5	ng	114488	5	14.045	901839	20.0
Ethanol, 2-(tet...	14.527	5.0	ng	224811	5	14.045	901839	20.0
Octadecanal	14.974	5.0	ng	108015	6	15.521	427402	20.0
Octadecane	15.174	2.0	ng	43150	6	15.521	427402	20.0
unknown15.198	15.198	7.6	ng	163266	6	15.521	427402	20.0
Benzo[e]pyrene	15.392	4.1	ng	87509	6	15.521	427402	20.0
Octacosane	16.004	3.3	ng	71323	6	15.521	427402	20.0
Cholest-5-ene, ...	17.609	7.4	ng	158091	6	15.521	427402	20.0
unknown17.851	17.851	4.7	ng	99669	6	15.521	427402	20.0