

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121024\
 Data File : BF140805.D
 Acq On : 10 Dec 2024 14:31
 Operator : RC/JU
 Sample : P5176-03 5X
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EO-03-12062024

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140805.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.504	576	580	606	rBV	86269	158292	5.56%	1.477%
2	6.516	748	752	774	rBV	80699	159011	5.58%	1.483%
3	6.863	806	811	828	rBV	253746	319895	11.23%	2.984%
4	7.428	903	907	916	rBV	59271	91627	3.22%	0.855%
5	8.145	1015	1029	1041	rBV	259219	375397	13.18%	3.502%
6	9.216	1207	1211	1220	rBV	133850	175540	6.16%	1.637%
7	9.898	1322	1327	1332	rBV	273899	348397	12.23%	3.250%
8	10.316	1392	1398	1403	rBV	22093	32727	1.15%	0.305%
9	10.698	1458	1463	1472	rVB	64906	98136	3.44%	0.915%
10	10.792	1475	1479	1487	rVB	24705	43268	1.52%	0.404%
11	11.392	1576	1581	1591	rBV2	313080	494825	17.37%	4.616%
12	11.698	1630	1633	1637	rVV	43478	53010	1.86%	0.494%
13	11.775	1641	1646	1651	rVB	755884	946151	33.21%	8.826%
14	11.922	1663	1671	1677	rBV4	31758	78120	2.74%	0.729%
15	12.010	1683	1686	1693	rVB2	18145	30644	1.08%	0.286%
16	12.080	1694	1698	1704	rBV2	18697	35575	1.25%	0.332%
17	12.463	1757	1763	1765	rBV	1946186	2848980	100.00%	26.575%
18	12.480	1765	1766	1773	rVV	1957163	2219847	77.92%	20.707%
19	12.563	1777	1780	1784	rVV	382223	481200	16.89%	4.489%
20	12.610	1784	1788	1801	rVV	166956	330497	11.60%	3.083%
21	12.839	1823	1827	1834	rVB	131596	190734	6.69%	1.779%
22	12.974	1846	1850	1854	rBV	178100	220004	7.72%	2.052%
23	14.045	2027	2032	2044	rVB2	281825	475050	16.67%	4.431%
24	14.169	2049	2053	2056	rBV	69539	98271	3.45%	0.917%
25	14.204	2056	2059	2063	rBV	89057	111281	3.91%	1.038%
26	15.545	2283	2287	2300	rVB	164588	304007	10.67%	2.836%

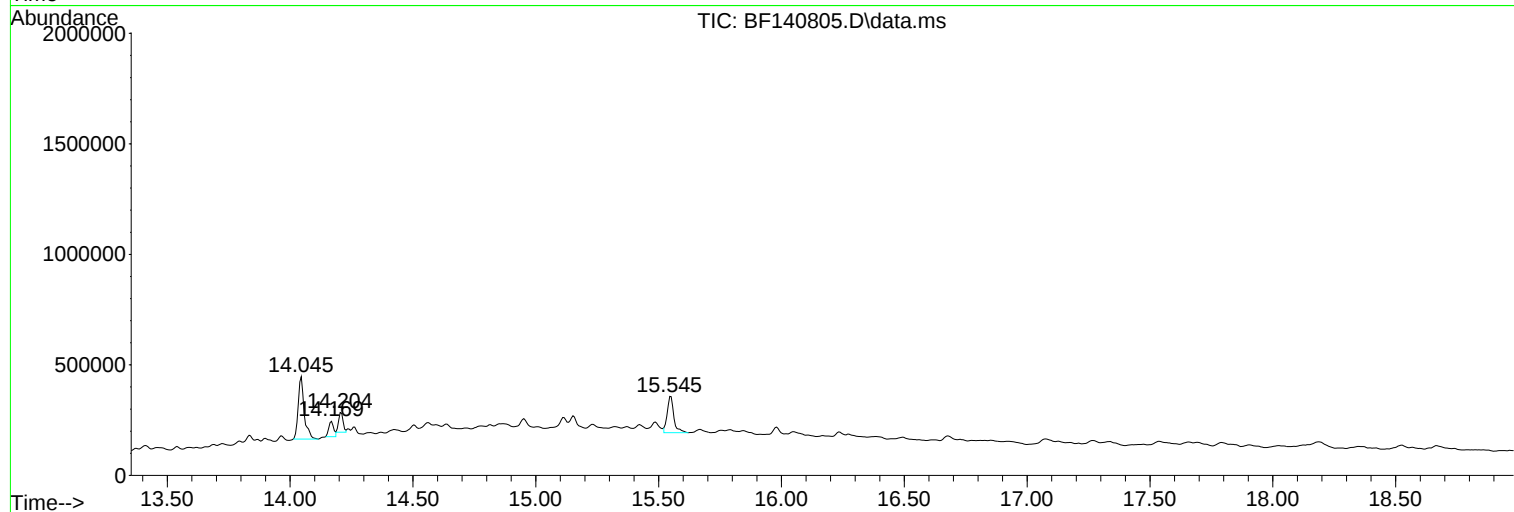
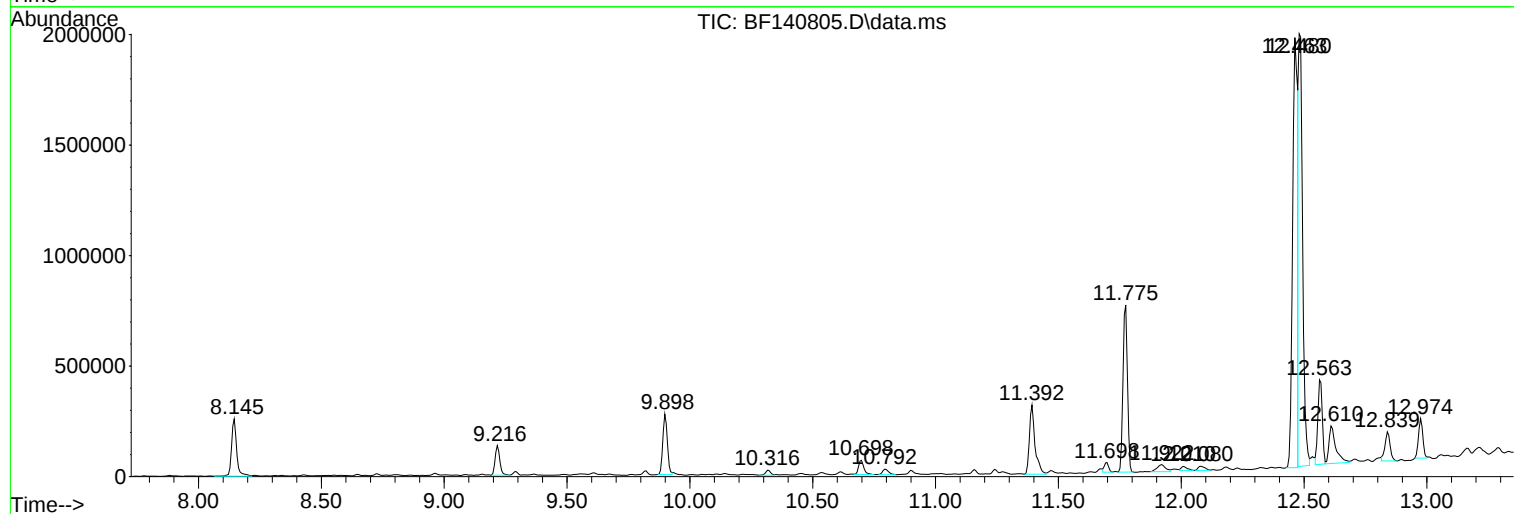
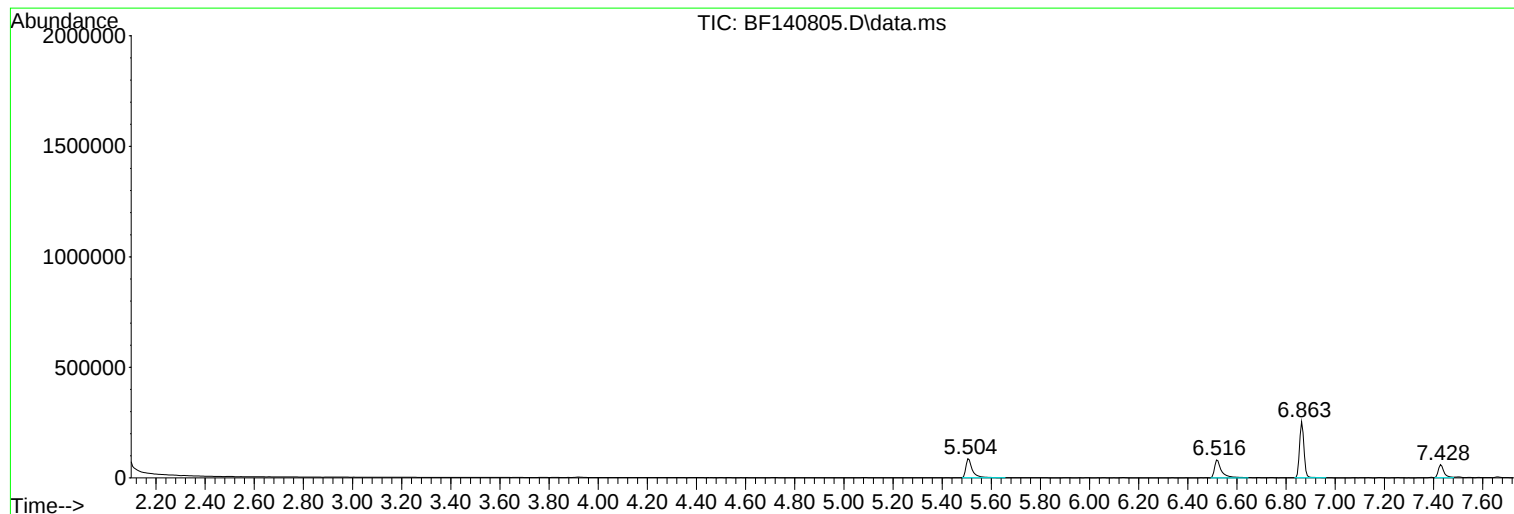
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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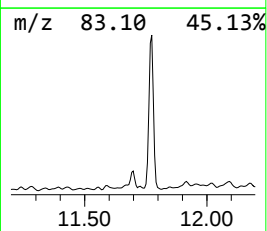
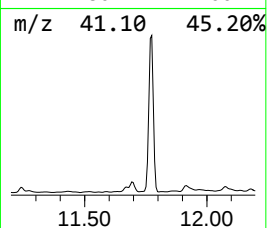
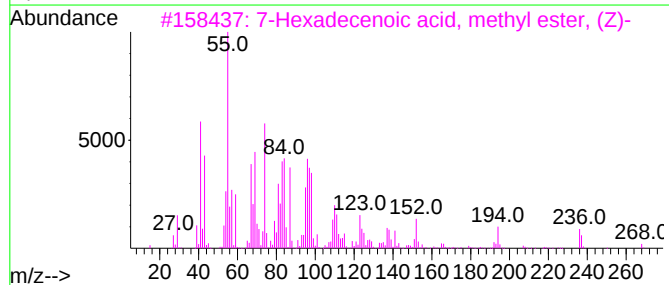
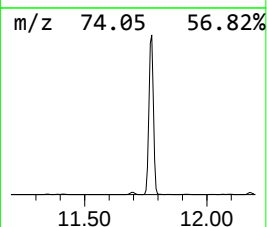
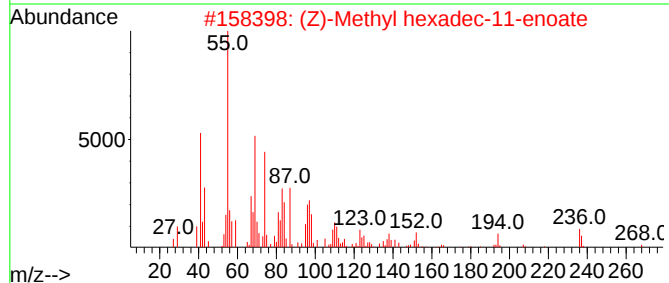
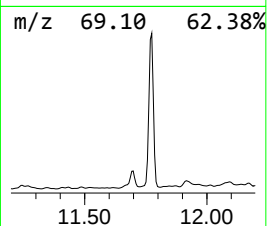
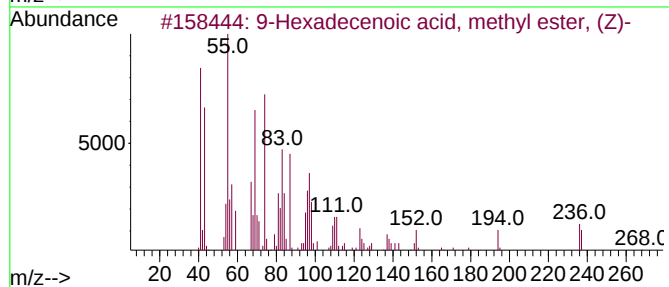
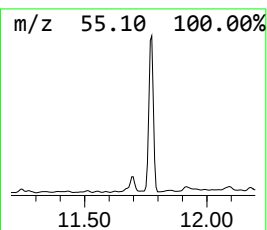
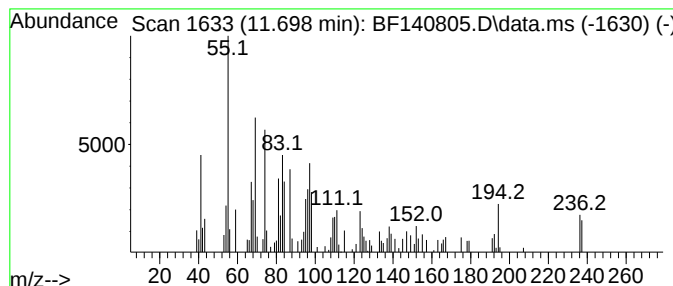
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 9-Hexadecenoic acid, methyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.698	2.14 ng	53010	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	83
2			(Z)-Methyl hexadec-11-enoate	268	C17H32O2	000822-05-9	74
3			7-Hexadecenoic acid, methyl este...	268	C17H32O2	056875-67-3	64
4			Palmitoleic acid	254	C16H30O2	000373-49-9	52
5			Methyl (Z)-10-pentadecenoate	254	C16H30O2	1000426-92-2	49



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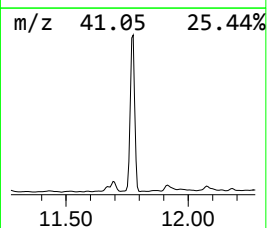
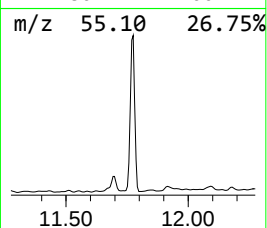
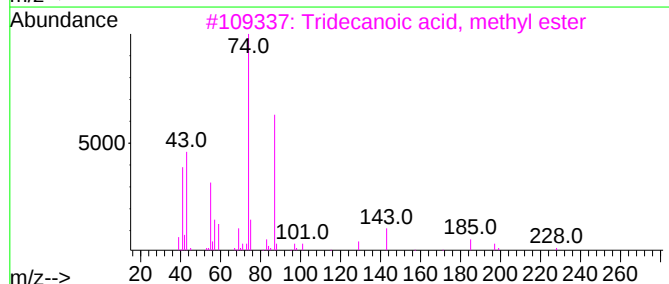
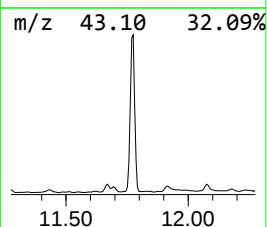
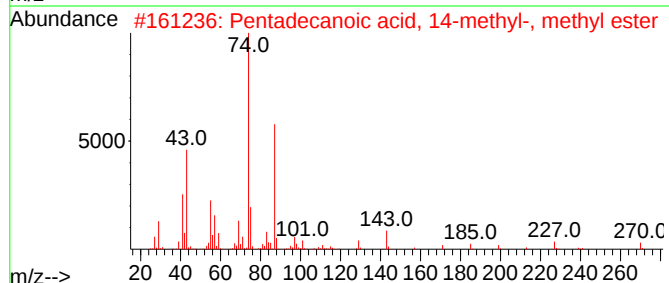
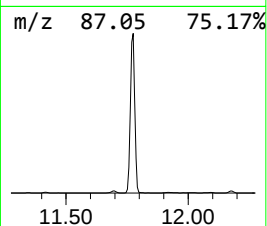
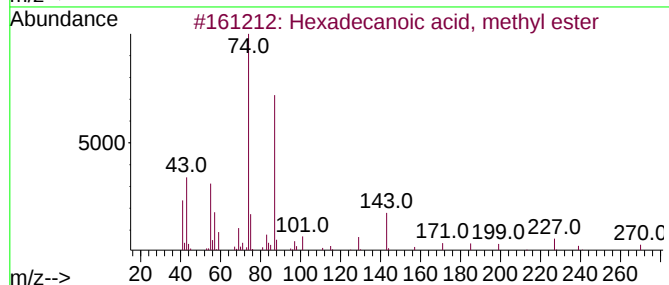
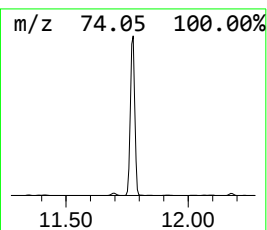
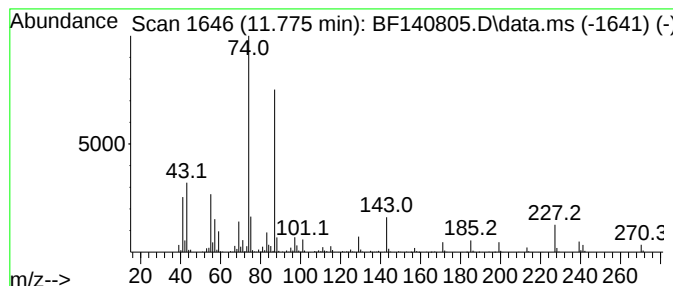
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.775	38.24 ng	946151	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	92
3			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
4			Hexadecanoic acid, 2-methyl-	270	C17H34O2	027147-71-3	87
5			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86



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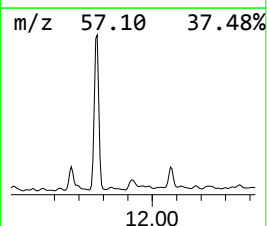
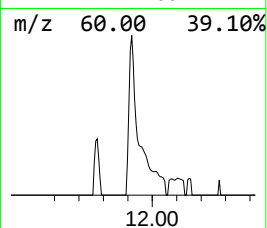
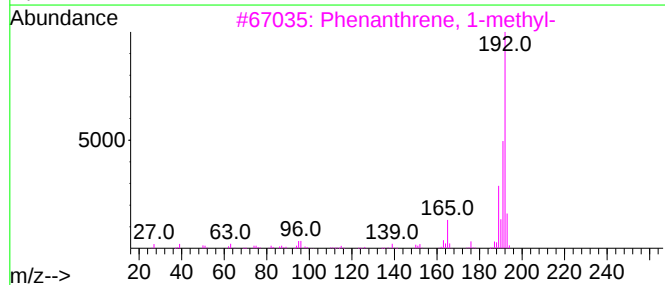
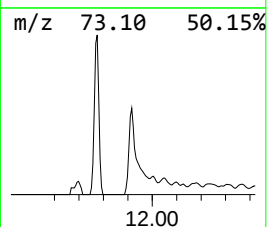
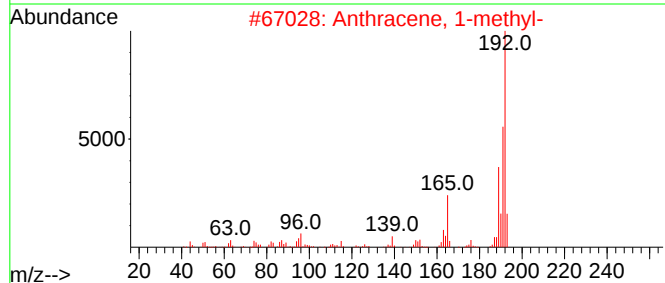
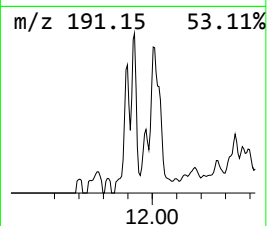
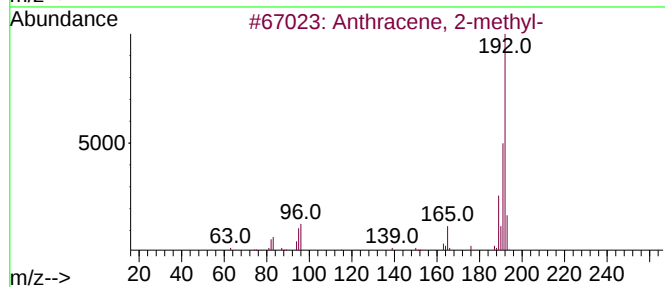
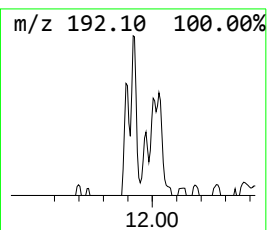
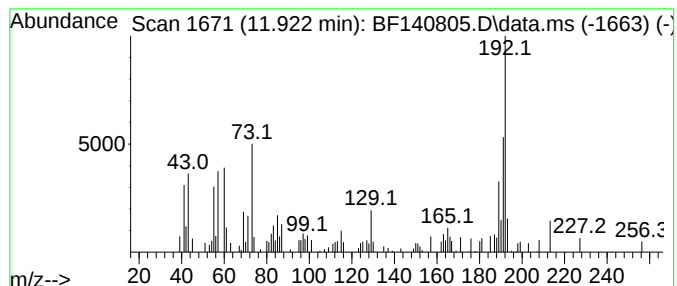
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Anthracene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	3.16 ng	78120	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 2-methyl-	192	C15H12	000613-12-7	62
2			Anthracene, 1-methyl-	192	C15H12	000610-48-0	55
3			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	55
4			Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	55
5			Anthracene, 9-methyl-	192	C15H12	000779-02-2	49



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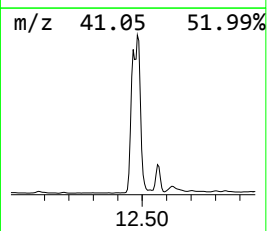
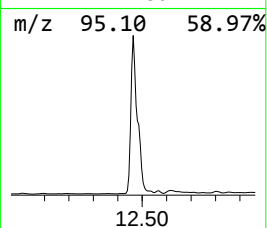
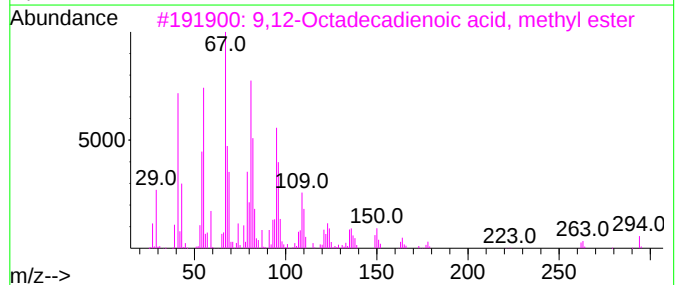
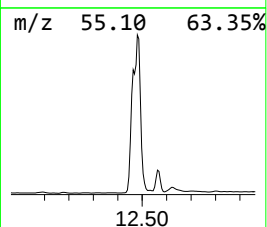
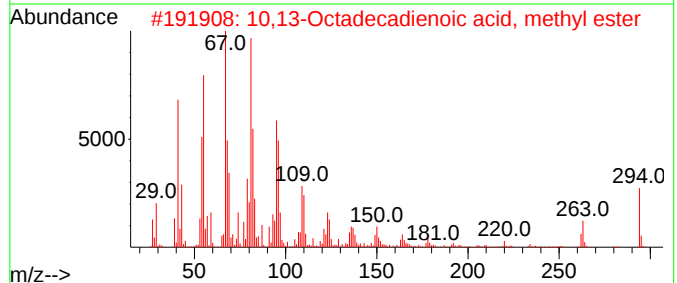
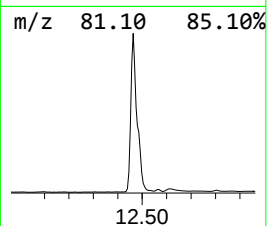
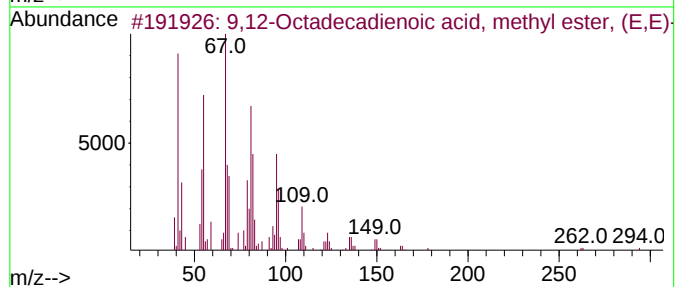
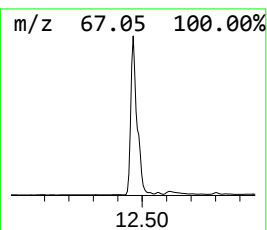
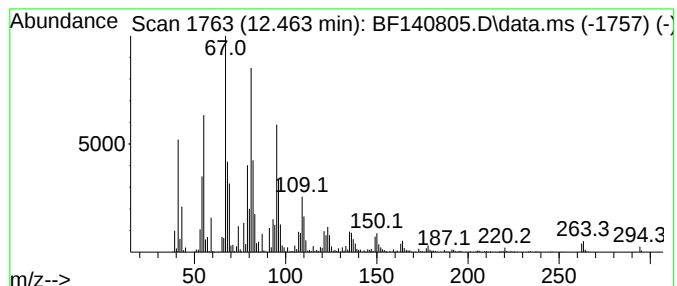
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Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.463	115.15 ng	2848980	Phenanthrene-d10	11.392	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
4	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
5	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99



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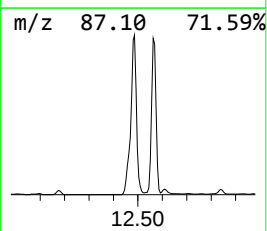
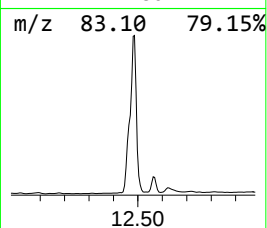
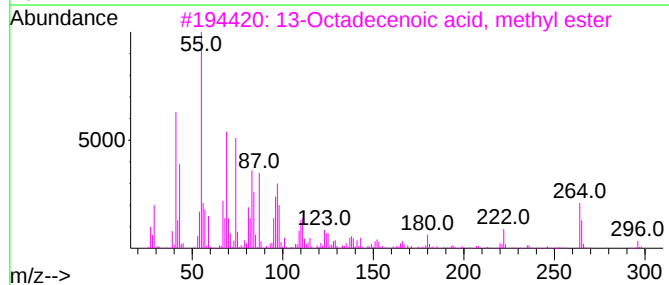
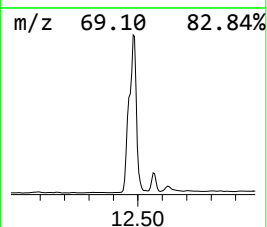
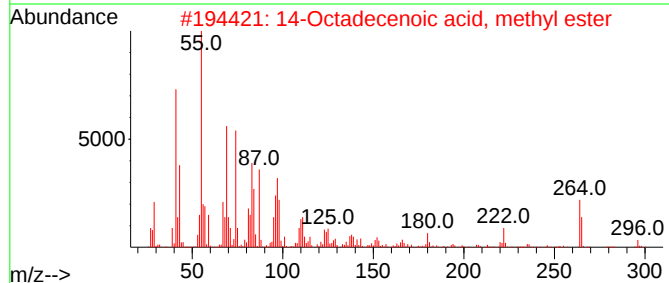
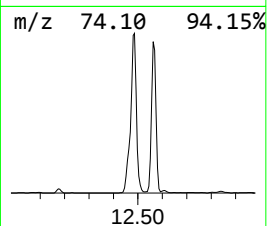
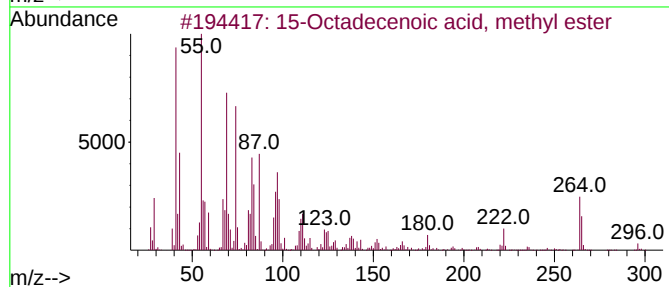
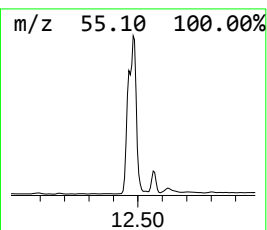
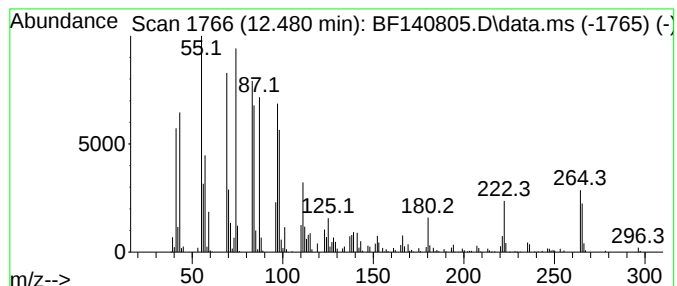
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Peak Number 5 15-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.480	89.72 ng	2219850	Phenanthrene-d10	11.392	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	90
2	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	90
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	90
4	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	90
5	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	90



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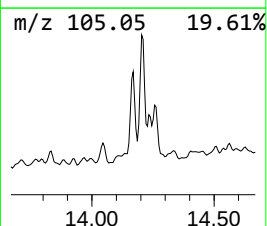
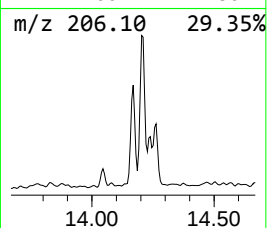
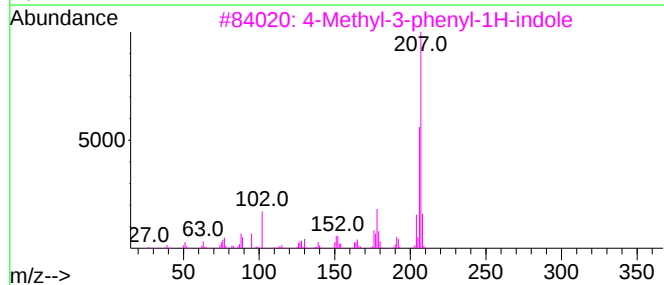
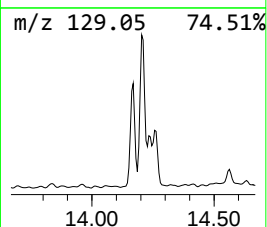
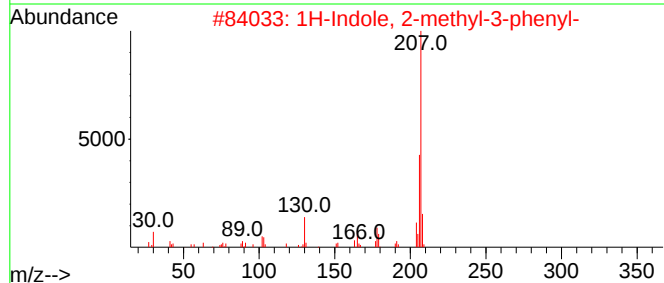
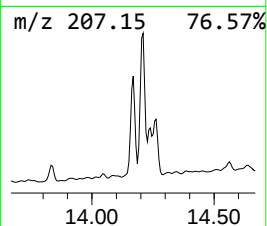
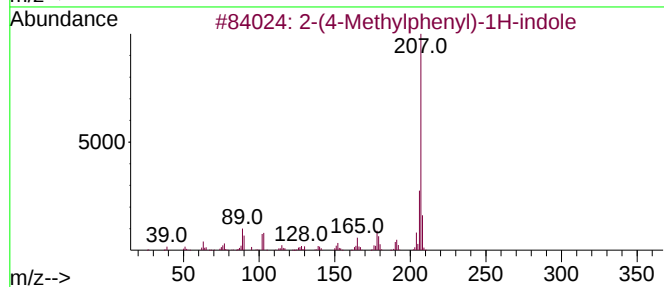
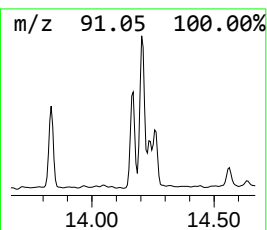
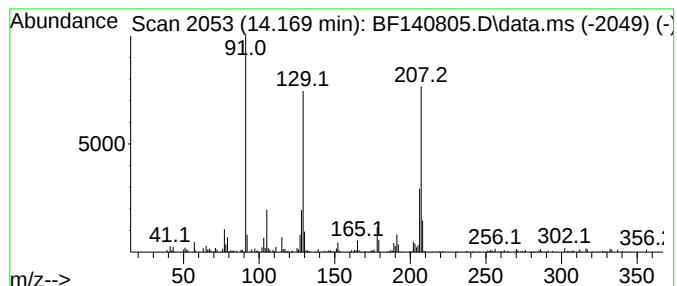
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown14.169 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.169	4.14 ng	98271	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(4-Methylphenyl)-1H-indole			207	C15H13N	055577-25-8	46
2	1H-Indole, 2-methyl-3-phenyl-			207	C15H13N	004757-69-1	41
3	4-Methyl-3-phenyl-1H-indole			207	C15H13N	180271-54-9	41
4	5-Methyl-2-phenylindolizine			207	C15H13N	036944-99-7	38
5	(2,3-Diphenylcyclopropyl)methyl ...			332	C22H20OS	131758-71-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121024\
Data File : BF140805.D
Acq On : 10 Dec 2024 14:31
Operator : RC/JU
Sample : P5176-03 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

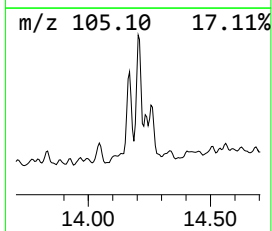
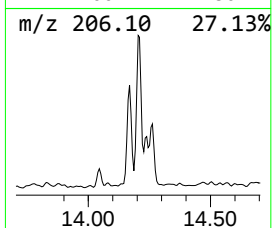
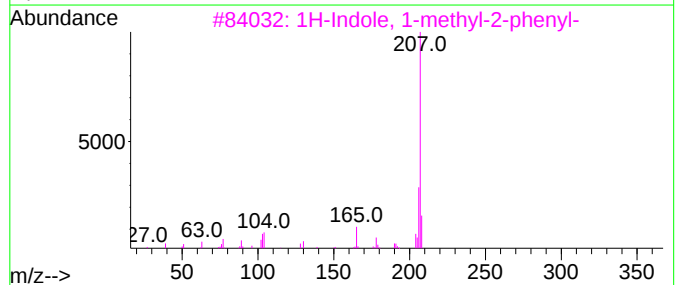
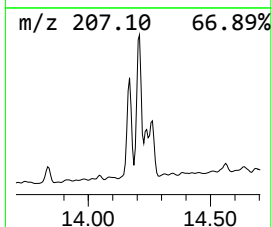
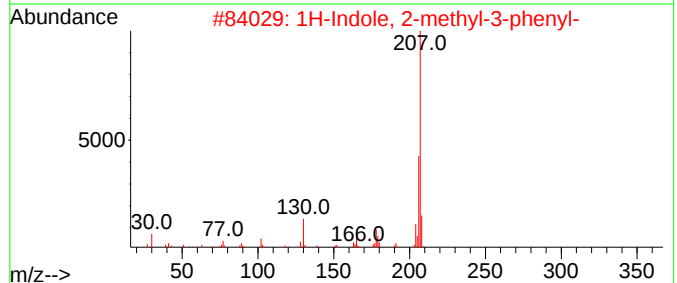
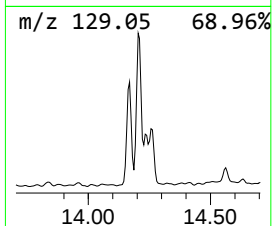
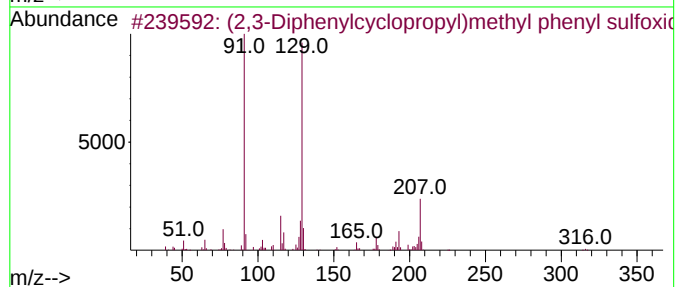
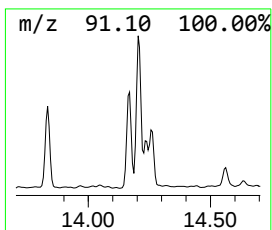
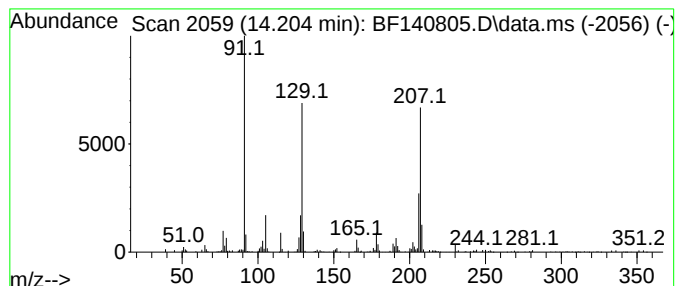
Instrument :
BNA_F
ClientSampleId :
EO-03-12062024

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

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

Peak Number 7 (2,3-Diphenylcyclopropyl)me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.204	4.69 ng	111281	Chrysene-d12		14.045	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	(2,3-Diphenylcyclopropyl)methyl ...		332	C22H20O5	131758-71-9	72
2	1H-Indole, 2-methyl-3-phenyl-		207	C15H13N	004757-69-1	46
3	1H-Indole, 1-methyl-2-phenyl-		207	C15H13N	003558-24-5	45
4	2-(4-Methylphenyl)-1H-indole		207	C15H13N	055577-25-8	42
5	1-benzylindole		207	C15H13N	1000334-31-3	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121024\
Data File : BF140805.D
Acq On : 10 Dec 2024 14:31
Operator : RC/JU
Sample : P5176-03 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EO-03-12062024

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

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
9-Hexadecenoic ...	11.698	2.1	ng	53010	4	11.392	494825	20.0
Hexadecanoic ac...	11.775	38.2	ng	946151	4	11.392	494825	20.0
Anthracene, 2-m...	11.922	3.2	ng	78120	4	11.392	494825	20.0
9,12-Octadecadi...	12.463	115.2	ng	2848980	4	11.392	494825	20.0
15-Octadecenoic...	12.480	89.7	ng	2219850	4	11.392	494825	20.0
unknown14.169	14.169	4.1	ng	98271	5	14.045	475050	20.0
(2,3-Diphenylcy...	14.204	4.7	ng	111281	5	14.045	475050	20.0