

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092823\
 Data File : BF135501.D
 Acq On : 28 Sep 2023 19:08
 Operator : CG\JU
 Sample : 04604-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TR-04-092523

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-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135501.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.987	489	493	501	rVB	31233	42962	1.25%	0.121%
2	5.387	557	561	584	rBV	3275275	3439483	100.00%	9.724%
3	6.398	729	733	758	rBV	3398299	3414790	99.28%	9.655%
4	6.586	761	765	776	rBV	73725	112509	3.27%	0.318%
5	6.745	789	792	796	rBV	1983918	1613832	46.92%	4.563%
6	7.310	884	888	891	rBV	2381109	2135253	62.08%	6.037%
7	7.333	891	892	896	rVB	63554	55150	1.60%	0.156%
8	8.022	1003	1009	1013	rBV	2179067	2007541	58.37%	5.676%
9	8.310	1054	1058	1065	rBV7	27061	50039	1.45%	0.141%
10	8.445	1077	1081	1082	rBV	38114	38132	1.11%	0.108%
11	8.616	1106	1110	1113	rBV	89117	84589	2.46%	0.239%
12	9.045	1180	1183	1188	rBV3	47293	46235	1.34%	0.131%
13	9.098	1188	1192	1196	rBV	3310685	3120773	90.73%	8.823%
14	9.180	1202	1206	1209	rBV	115843	105020	3.05%	0.297%
15	9.222	1209	1213	1216	rBV	1338795	1170727	34.04%	3.310%
16	9.374	1236	1239	1243	rBV4	57385	44974	1.31%	0.127%
17	9.498	1258	1260	1262	rVB2	43492	34491	1.00%	0.098%
18	9.639	1281	1284	1288	rBV3	36026	44751	1.30%	0.127%
19	9.710	1293	1296	1300	rVB	88170	67870	1.97%	0.192%
20	9.780	1304	1308	1311	rVV	2115573	1801467	52.38%	5.093%
21	9.810	1311	1313	1317	rVB	41884	36801	1.07%	0.104%
22	9.986	1341	1343	1347	rVB4	38266	48244	1.40%	0.136%
23	10.033	1347	1351	1354	rBV4	29544	43069	1.25%	0.122%
24	10.210	1378	1381	1384	rVB	71279	55925	1.63%	0.158%
25	10.433	1414	1419	1423	rVB3	31244	40694	1.18%	0.115%
26	10.574	1439	1443	1455	rVB	1606972	1607895	46.75%	4.546%
27	10.686	1459	1462	1470	rVB3	72706	103784	3.02%	0.293%
28	10.757	1470	1474	1475	rBV2	38854	39864	1.16%	0.113%
29	10.851	1487	1490	1493	rBV2	40707	47704	1.39%	0.135%
30	11.016	1515	1518	1526	rVB7	27527	51292	1.49%	0.145%
31	11.133	1536	1538	1541	rBV	39914	38556	1.12%	0.109%
32	11.169	1541	1544	1548	rVB2	45894	52319	1.52%	0.148%
33	11.268	1558	1561	1564	rBV	1746459	1590836	46.25%	4.498%
34	11.292	1564	1565	1569	rVV	308665	221295	6.43%	0.626%
35	11.345	1572	1574	1577	rVB	70748	62988	1.83%	0.178%
36	11.516	1600	1603	1608	rVB	36254	39808	1.16%	0.113%

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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-BF091123.M
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37	11.668	1626	1629	1634	rVB	232969	178543	5.19%	0.505%
38	11.774	1644	1647	1649	rBV	53669	52856	1.54%	0.149%
39	11.804	1649	1652	1660	rVV	532270	587013	17.07%	1.660%
40	11.886	1663	1666	1669	rBV	99576	91296	2.65%	0.258%
41	12.327	1738	1741	1743	rBV	60253	57165	1.66%	0.162%
42	12.357	1743	1746	1748	rVV	872067	711296	20.68%	2.011%
43	12.380	1748	1750	1754	rVB	475045	404816	11.77%	1.145%
44	12.463	1762	1764	1766	rBV	75276	64623	1.88%	0.183%
45	12.492	1766	1769	1772	rVV	719166	682712	19.85%	1.930%
46	12.592	1783	1786	1792	rBV2	139531	187272	5.44%	0.529%
47	12.721	1802	1808	1811	rBV	696485	768894	22.35%	2.174%
48	12.863	1828	1832	1836	rBV	2472886	2293229	66.67%	6.484%
49	13.027	1857	1860	1861	rBV2	45582	49303	1.43%	0.139%
50	13.051	1862	1864	1867	rVB	124511	103352	3.00%	0.292%
51	13.098	1870	1872	1873	rVV	49575	36512	1.06%	0.103%
52	13.115	1873	1875	1878	rVB	103200	87258	2.54%	0.247%
53	13.157	1879	1882	1884	rBV2	69890	68981	2.01%	0.195%
54	13.251	1895	1898	1901	rBV	48924	49473	1.44%	0.140%
55	13.280	1901	1903	1905	rBV	45229	41444	1.20%	0.117%
56	13.674	1968	1970	1972	rBV	66511	57166	1.66%	0.162%
57	13.727	1977	1979	1981	rBV	55560	52004	1.51%	0.147%
58	13.774	1984	1987	1995	rVV3	268892	389114	11.31%	1.100%
59	13.927	2008	2013	2016	rBV2	1671378	1908886	55.50%	5.397%
60	13.951	2016	2017	2021	rVB	414479	286106	8.32%	0.809%
61	14.033	2029	2031	2034	rVB	95577	72576	2.11%	0.205%
62	14.962	2186	2189	2193	rBV	335880	517441	15.04%	1.463%
63	15.262	2237	2240	2247	rVB	204746	249932	7.27%	0.707%
64	15.327	2247	2251	2256	rVV	277347	372650	10.83%	1.054%
65	15.386	2257	2261	2273	rVB	961380	1436187	41.76%	4.060%

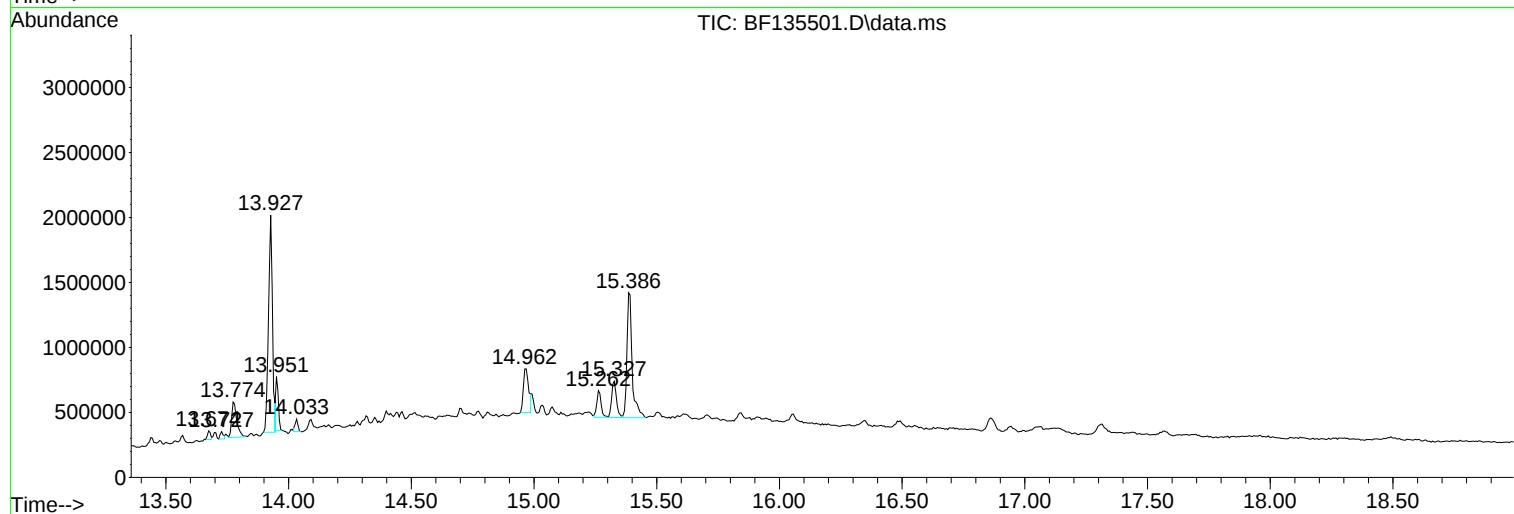
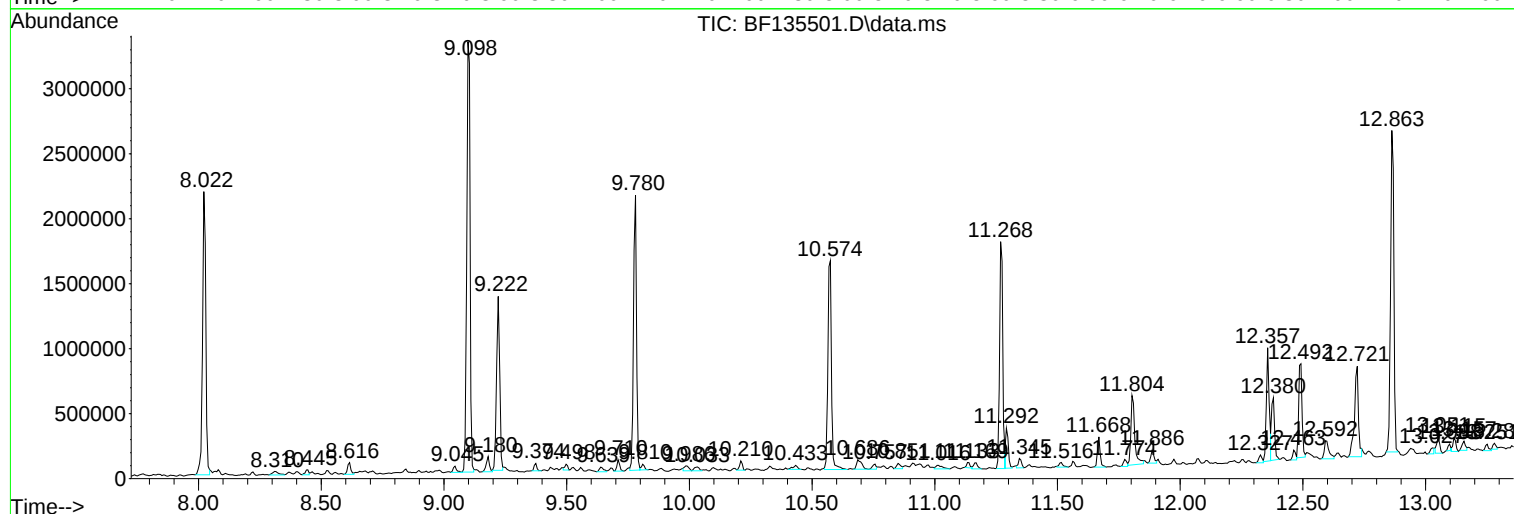
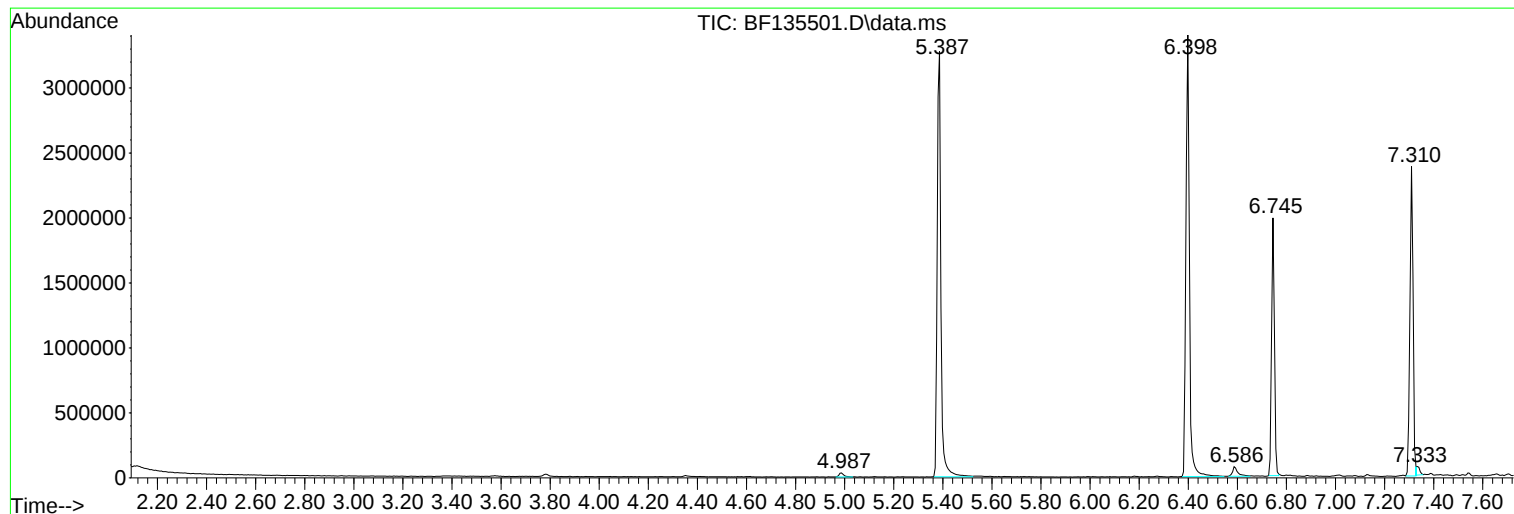
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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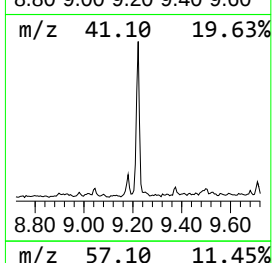
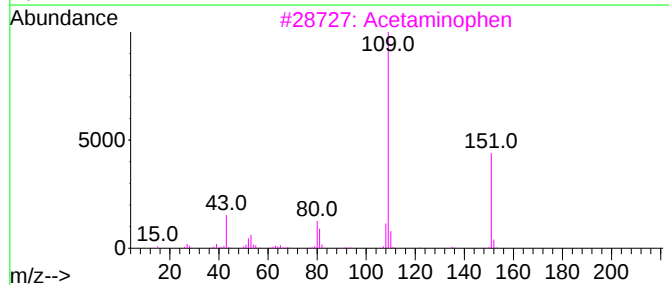
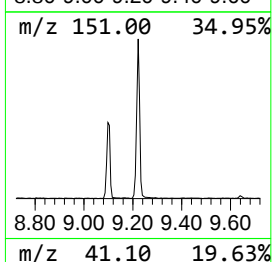
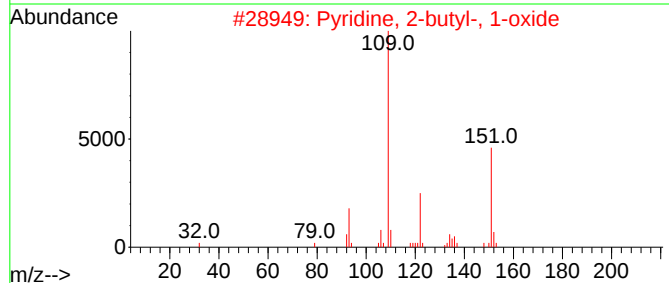
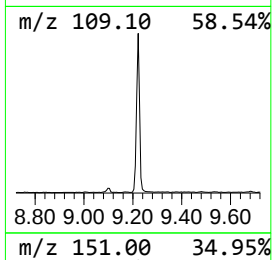
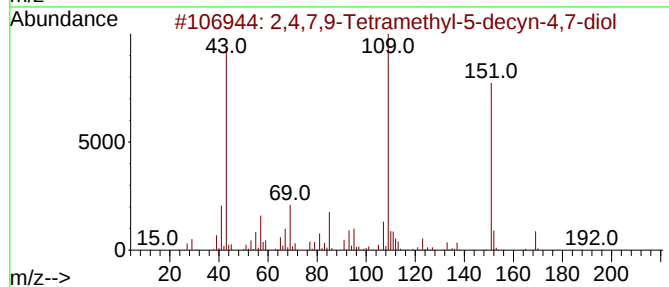
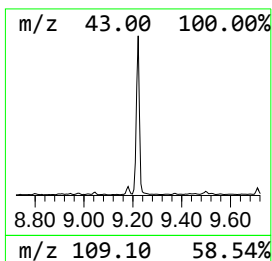
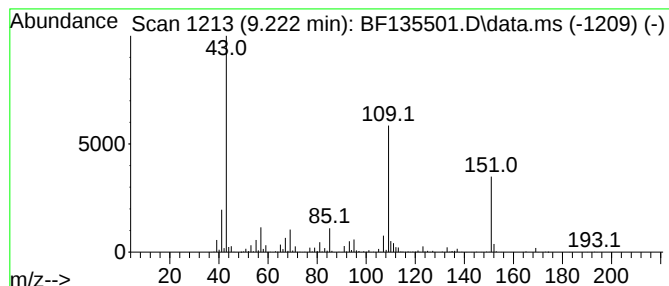
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.222	13.00 ng	1170730	Acenaphthene-d10	9.780

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	87	
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53	
3	Acetaminophen	151	C8H9NO2	000103-90-2	47	
4	Metacetamol	151	C8H9NO2	000621-42-1	47	
5	benzenamine, 3-[(tetrahydro-2H-p...	193	C11H15NO2	1010400-28-1	43	



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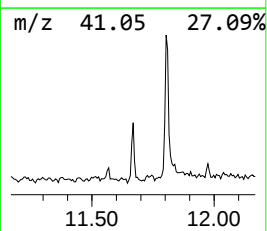
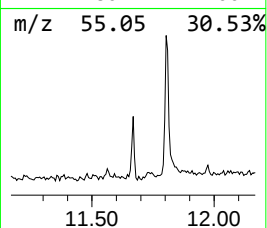
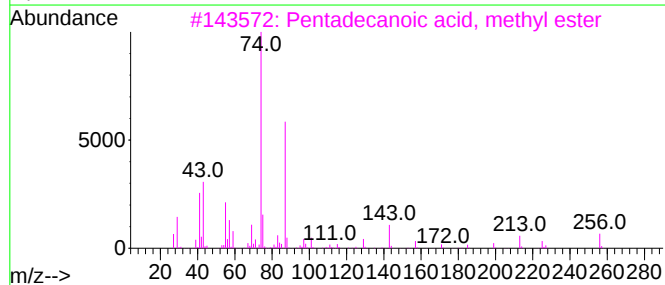
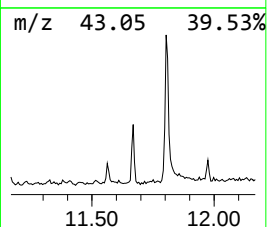
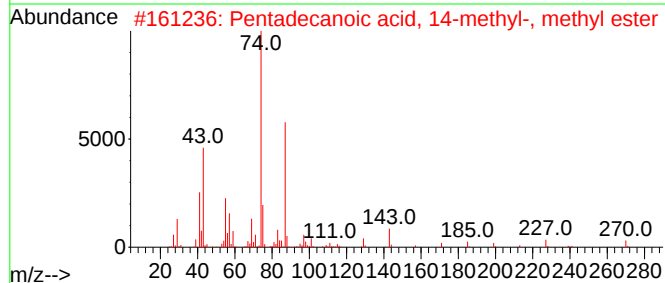
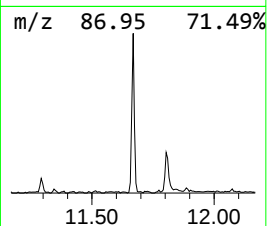
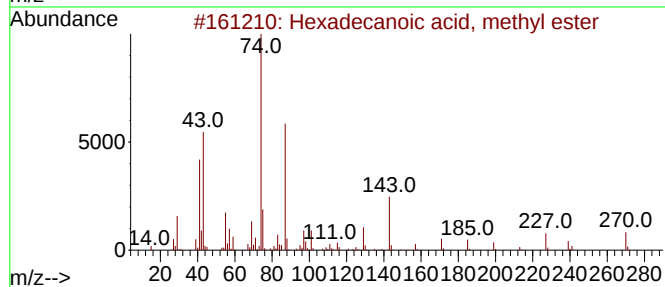
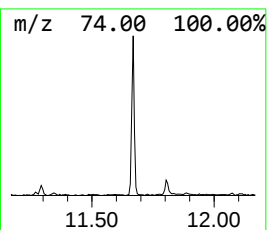
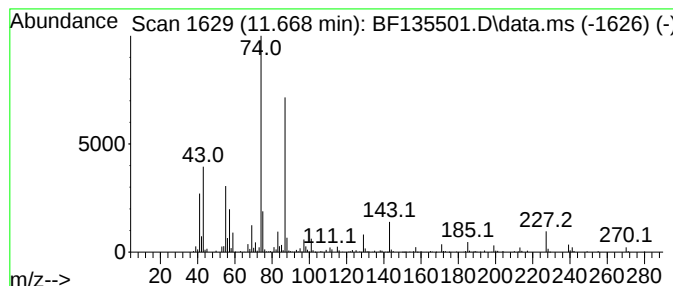
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.669	2.24 ng	178543	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	96
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	87
3			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
4			Hexadecanoic acid, 2-methyl-	270	C17H34O2	027147-71-3	83
5			Methyl tetradecanoate	242	C15H30O2	000124-10-7	80



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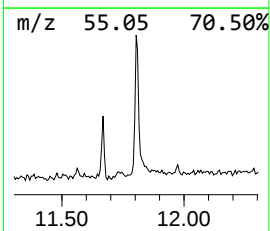
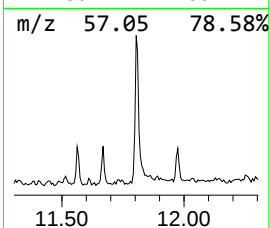
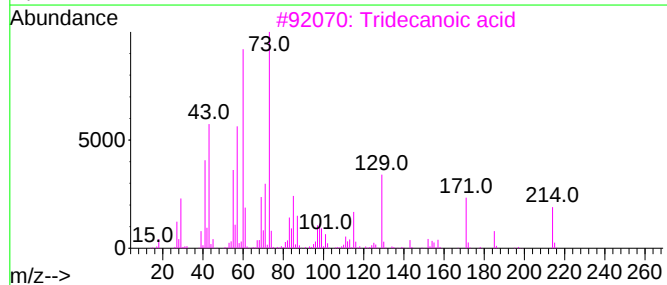
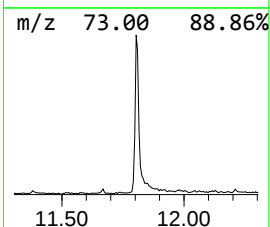
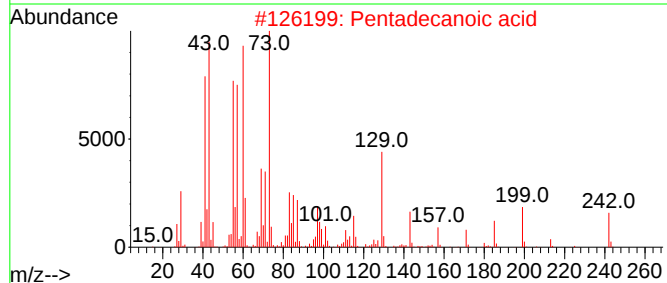
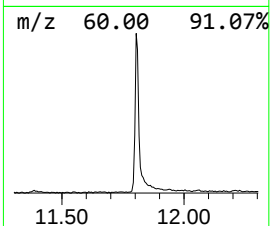
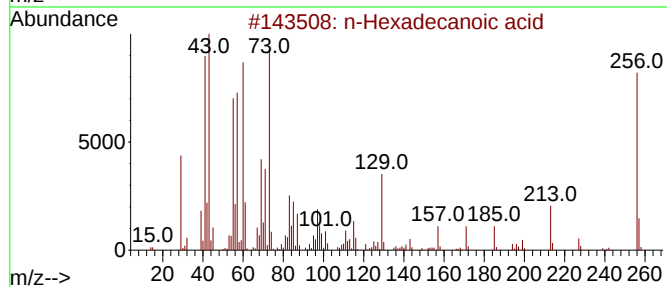
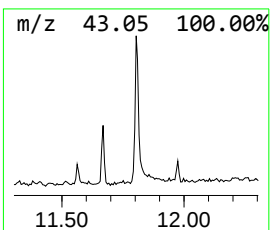
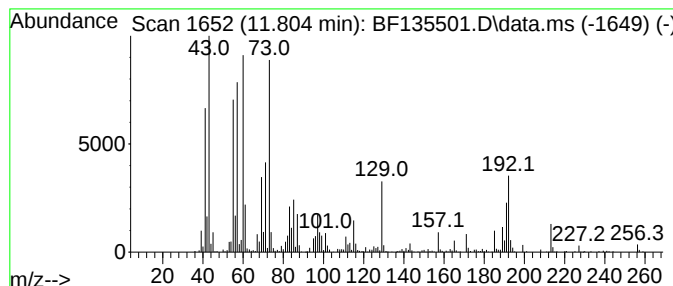
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	7.38 ng	587013	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	70
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



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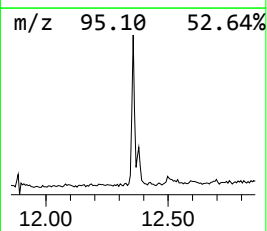
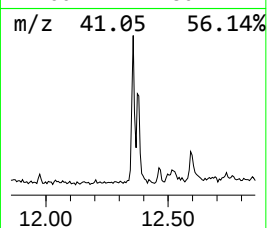
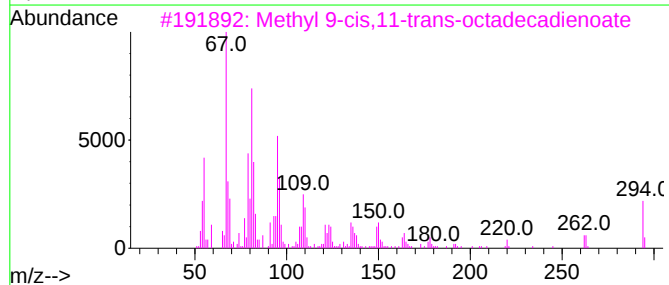
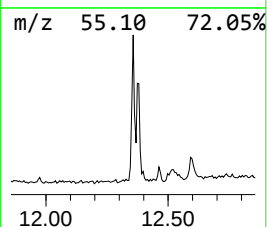
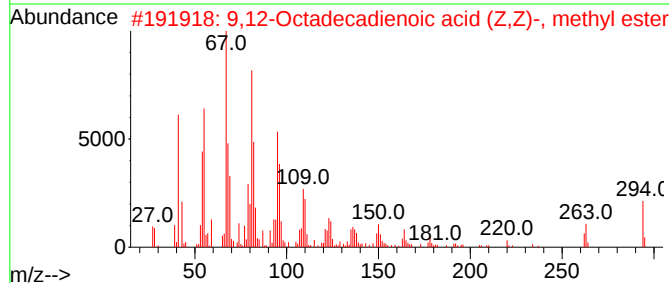
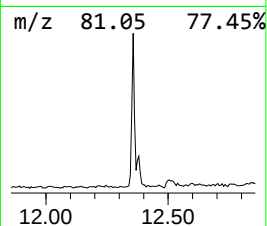
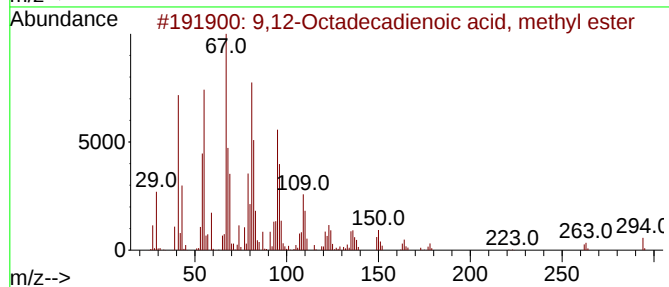
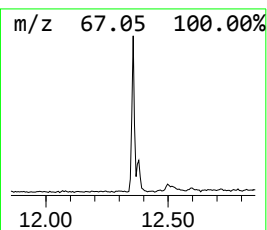
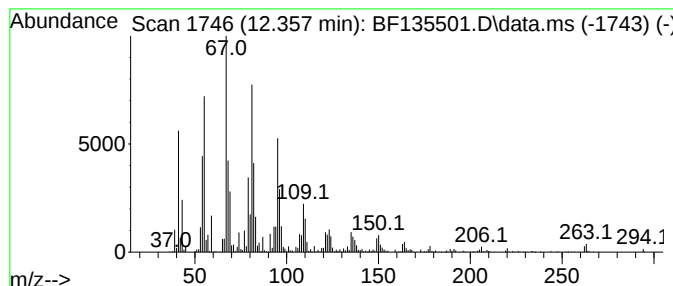
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.357	8.94 ng	711296	Phenanthrene-d10		11.269	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...		294	C19H34O2	002462-85-3	99
2	9,12-Octadecadienoic acid (Z,Z)-...		294	C19H34O2	000112-63-0	99
3	Methyl 9-cis,11-trans-octadecadi...		294	C19H34O2	013058-52-1	99
4	10,13-Octadecadienoic acid, meth...		294	C19H34O2	056554-62-2	99
5	9,12-Octadecadienoic acid, methy...		294	C19H34O2	002566-97-4	98



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092823\
Data File : BF135501.D
Acq On : 28 Sep 2023 19:08
Operator : CG\JU
Sample : 04604-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

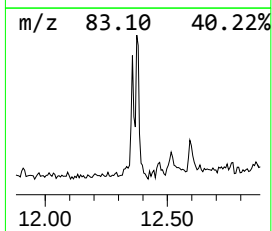
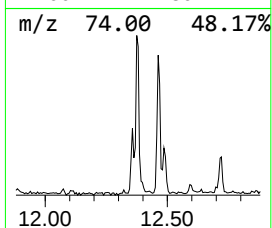
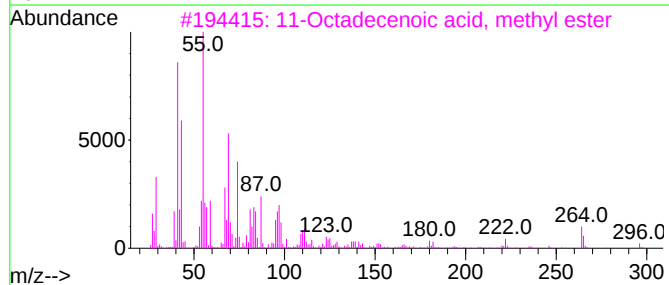
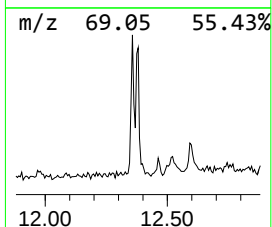
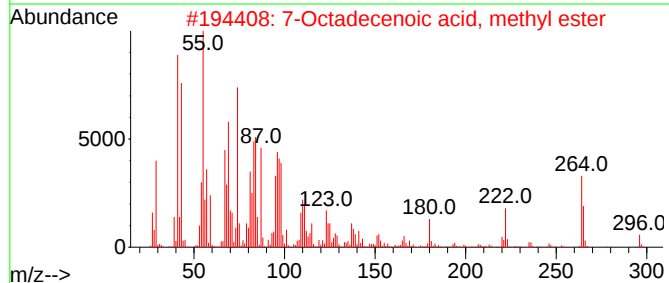
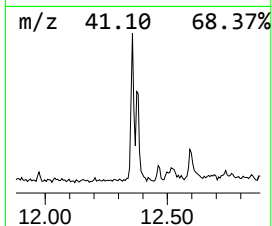
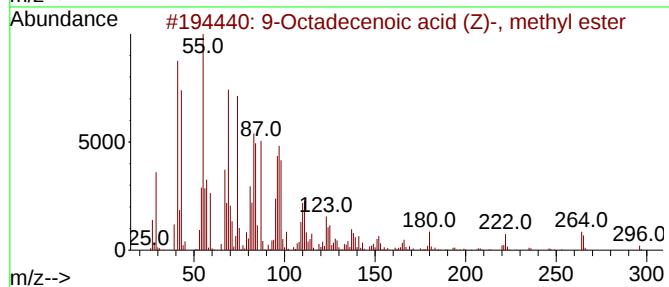
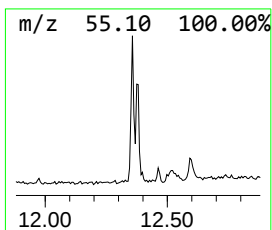
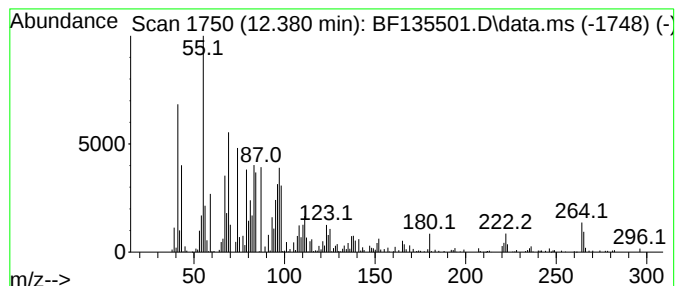
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ClientSampleId :
TR-04-092523

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 9-Octadecenoic acid (Z)-, m... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.380	5.09 ng	404816	Phenanthrene-d10	11.269	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	7-Octadecenoic acid, methyl ester	296	C19H36O2	057396-98-2	99
3	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99
4	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	98
5	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	97



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092823\
Data File : BF135501.D
Acq On : 28 Sep 2023 19:08
Operator : CG\JU
Sample : 04604-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-092523

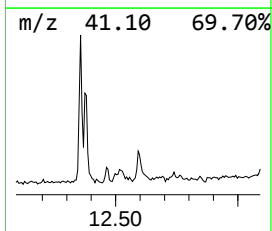
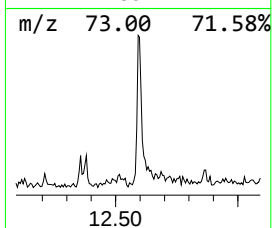
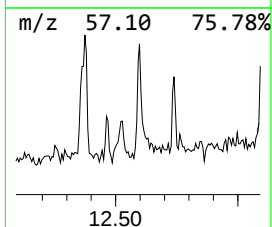
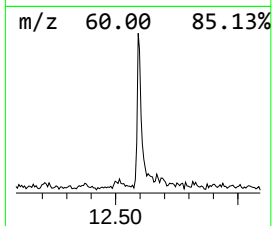
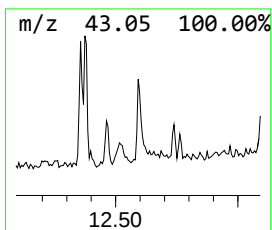
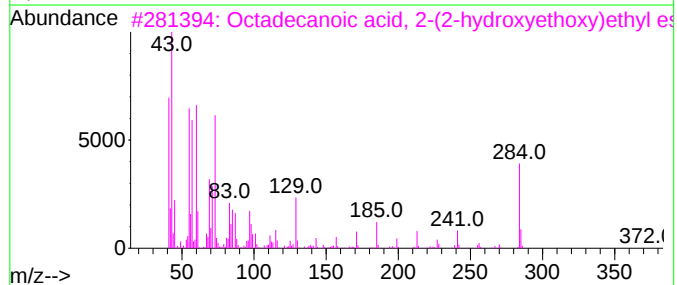
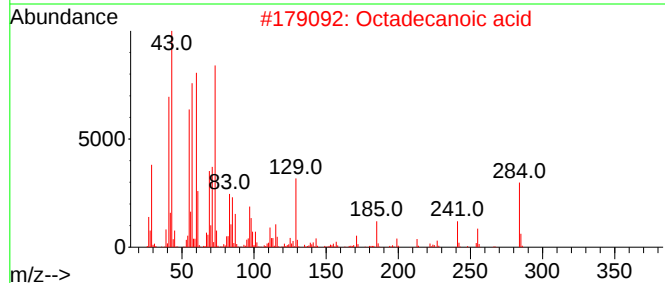
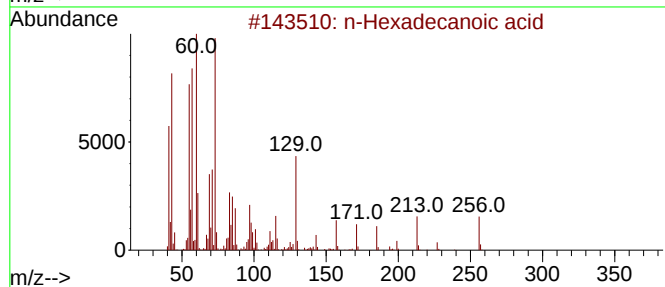
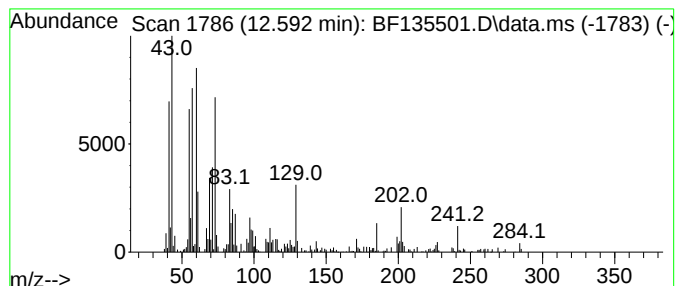
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.592	2.35 ng	187272	Phenanthrene-d10	11.269

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2		Octadecanoic acid	284	C18H36O2	000057-11-4	90
3		Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	74
4		n-Decanoic acid	172	C10H20O2	000334-48-5	53
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092823\
Data File : BF135501.D
Acq On : 28 Sep 2023 19:08
Operator : CG\JU
Sample : 04604-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-092523

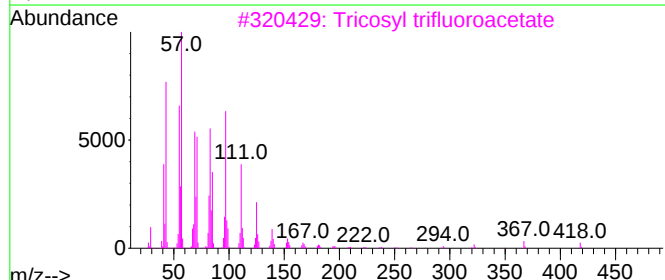
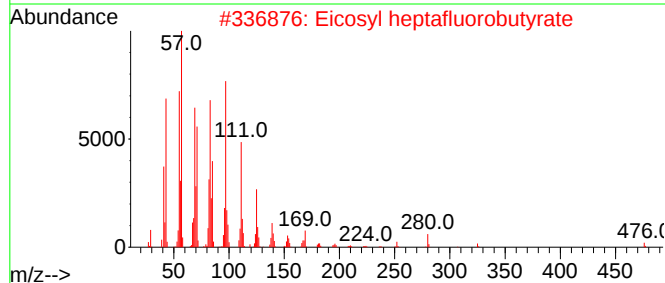
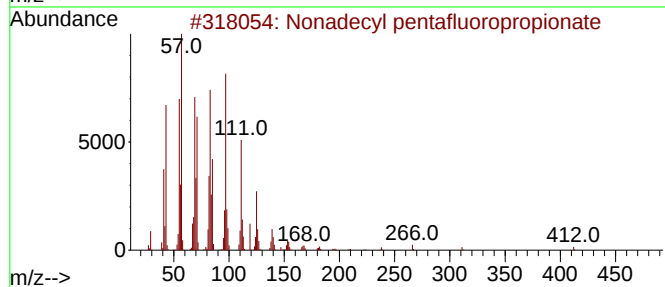
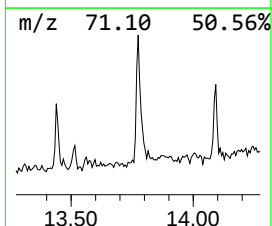
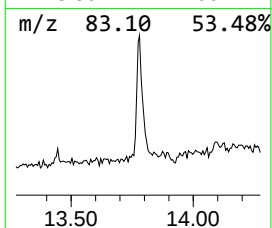
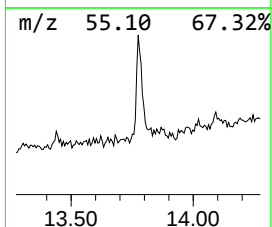
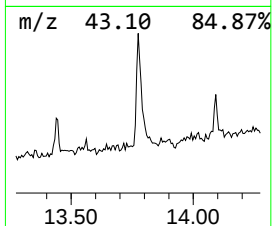
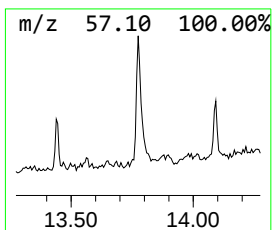
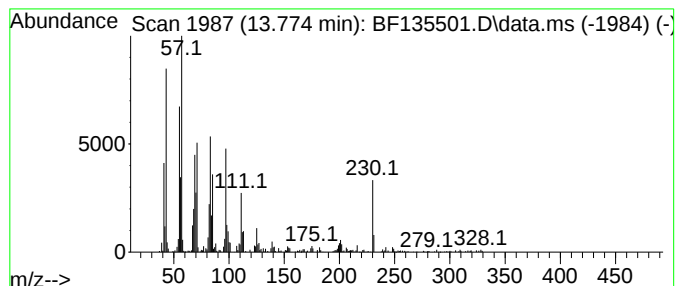
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecyl pentafluoropropio... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	4.08 ng	389114	Chrysene-d12	13.927

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	83
2			Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	83
3			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	83
4			Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	83
5			Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092823\
Data File : BF135501.D
Acq On : 28 Sep 2023 19:08
Operator : CG\JU
Sample : 04604-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-092523

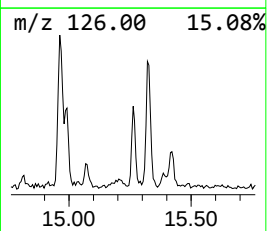
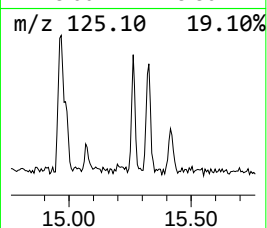
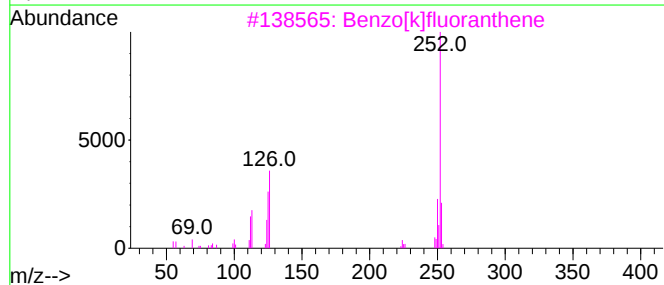
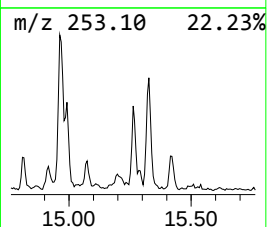
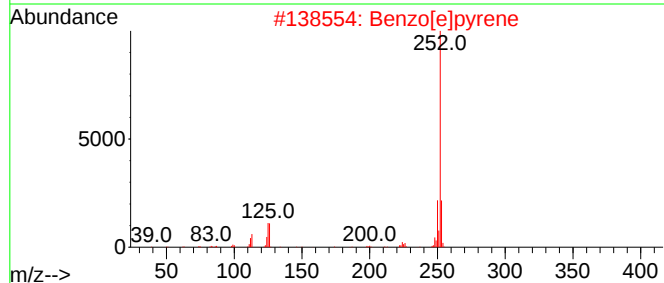
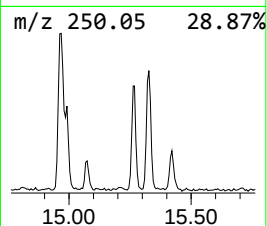
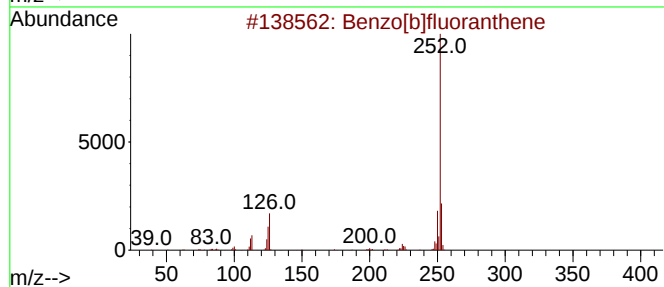
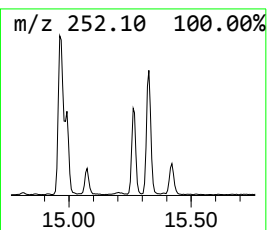
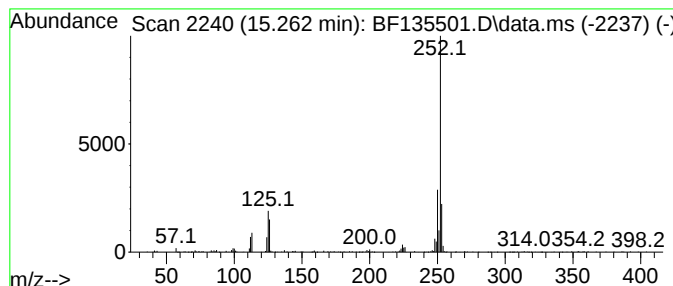
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.262	3.48 ng	249932	Perylene-d12	15.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]fluoranthene	252	C20H12	000205-99-2	98
2			Benzo[e]pyrene	252	C20H12	000192-97-2	98
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
5			Perylene	252	C20H12	000198-55-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092823\
Data File : BF135501.D
Acq On : 28 Sep 2023 19:08
Operator : CG\JU
Sample : 04604-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2,4,7,9-Tetrame...	9.222	13.0	ng	1170730	3	9.780	1801470	20.0
Hexadecanoic ac...	11.669	2.2	ng	178543	4	11.269	1590840	20.0
n-Hexadecanoic ...	11.804	7.4	ng	587013	4	11.269	1590840	20.0
9,12-Octadecadi...	12.357	8.9	ng	711296	4	11.269	1590840	20.0
9-Octadecenoic ...	12.380	5.1	ng	404816	4	11.269	1590840	20.0
Octadecanoic acid	12.592	2.4	ng	187272	4	11.269	1590840	20.0
Nonadecyl penta...	13.774	4.1	ng	389114	5	13.927	1908890	20.0
Benzo[e]pyrene	15.262	3.5	ng	249932	6	15.392	1436190	20.0