

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091423\
 Data File : BF135266.D
 Acq On : 14 Sep 2023 21:42
 Operator : CG\JU
 Sample : 04399-03
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 72-11985

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: BF135266.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	12	15	26	rVB2	20873	42572	1.46%	0.183%
2	5.016	492	498	509	rVB	44028	66915	2.29%	0.287%
3	5.404	559	564	567	rBV	2782698	2670006	91.26%	11.462%
4	6.410	730	735	738	rBV	2495385	2641875	90.30%	11.341%
5	6.763	791	795	798	rBV	860585	726478	24.83%	3.119%
6	7.328	886	891	894	rBV	1828594	1735477	59.32%	7.450%
7	8.039	1008	1012	1015	rBV	1126388	922330	31.53%	3.960%
8	9.122	1190	1196	1199	rBV	3355538	2925585	100.00%	12.559%
9	9.798	1306	1311	1314	rBV	1141539	940567	32.15%	4.038%
10	10.592	1442	1446	1449	rBV	1467165	1336413	45.68%	5.737%
11	11.292	1561	1565	1567	rBV	867348	820846	28.06%	3.524%
12	11.316	1567	1569	1572	rVV	261616	216271	7.39%	0.928%
13	11.363	1573	1577	1581	rVB	43698	44959	1.54%	0.193%
14	11.527	1600	1605	1613	rBV2	28776	46611	1.59%	0.200%
15	11.792	1646	1650	1653	rBV2	68478	68117	2.33%	0.292%
16	11.827	1653	1656	1661	rVV2	215891	217867	7.45%	0.935%
17	11.904	1666	1669	1672	rBV	67895	67260	2.30%	0.289%
18	12.122	1703	1706	1710	rVB	58757	52545	1.80%	0.226%
19	12.433	1756	1759	1762	rBV	36855	35526	1.21%	0.153%
20	12.510	1768	1772	1775	rBV	616889	536460	18.34%	2.303%
21	12.598	1785	1787	1789	rBV2	51557	46846	1.60%	0.201%
22	12.698	1801	1804	1806	rBV3	47252	49426	1.69%	0.212%
23	12.739	1806	1811	1814	rVB	511932	497631	17.01%	2.136%
24	12.886	1832	1836	1840	rVV	2184780	2053188	70.18%	8.814%
25	12.963	1843	1849	1852	rBV2	30664	48039	1.64%	0.206%
26	13.045	1860	1863	1865	rBV3	29847	36432	1.25%	0.156%
27	13.069	1865	1867	1871	rVB	60500	56322	1.93%	0.242%
28	13.139	1872	1879	1881	rBV2	43175	62553	2.14%	0.269%
29	13.174	1881	1885	1887	rBV	46168	45698	1.56%	0.196%
30	13.586	1952	1955	1959	rVB	43209	38785	1.33%	0.167%
31	13.692	1969	1973	1976	rBV	59382	68832	2.35%	0.295%
32	13.810	1988	1993	1999	rBV3	83028	165919	5.67%	0.712%
33	13.945	2010	2016	2019	rBV2	739170	1042080	35.62%	4.474%
34	13.974	2019	2021	2024	rVB	223508	179336	6.13%	0.770%
35	14.051	2031	2034	2036	rVB	70408	56227	1.92%	0.241%
36	14.333	2079	2082	2086	rVB4	50928	59301	2.03%	0.255%

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37	14.380	2086	2090	2092	rBV3	39287	48776	1.67%	0.209%
38	14.457	2100	2103	2106	rBV2	89884	88195	3.01%	0.379%
39	14.533	2109	2116	2117	rBV2	85291	146221	5.00%	0.628%
40	14.586	2122	2125	2129	rBV3	113748	162543	5.56%	0.698%
41	14.627	2130	2132	2134	rBV	46693	40636	1.39%	0.174%
42	14.715	2144	2147	2153	rVB	109852	204889	7.00%	0.880%
43	14.768	2153	2156	2160	rBV	61275	65587	2.24%	0.282%
44	14.874	2172	2174	2178	rVB2	39481	35445	1.21%	0.152%
45	14.986	2189	2193	2196	rBV	238969	333645	11.40%	1.432%
46	15.068	2204	2207	2210	rVB2	45944	42024	1.44%	0.180%
47	15.286	2241	2244	2250	rVB	149311	187063	6.39%	0.803%
48	15.351	2251	2255	2261	rBV	163754	217198	7.42%	0.932%
49	15.415	2261	2266	2270	rBV	502187	614927	21.02%	2.640%
50	15.657	2304	2307	2311	rVB3	50688	64898	2.22%	0.279%
51	15.892	2344	2347	2351	rVB2	57439	77208	2.64%	0.331%
52	16.704	2480	2485	2492	rVB8	34852	75665	2.59%	0.325%
53	16.886	2511	2516	2527	rVB2	70803	157800	5.39%	0.677%
54	17.333	2588	2592	2601	rVB2	54847	109884	3.76%	0.472%

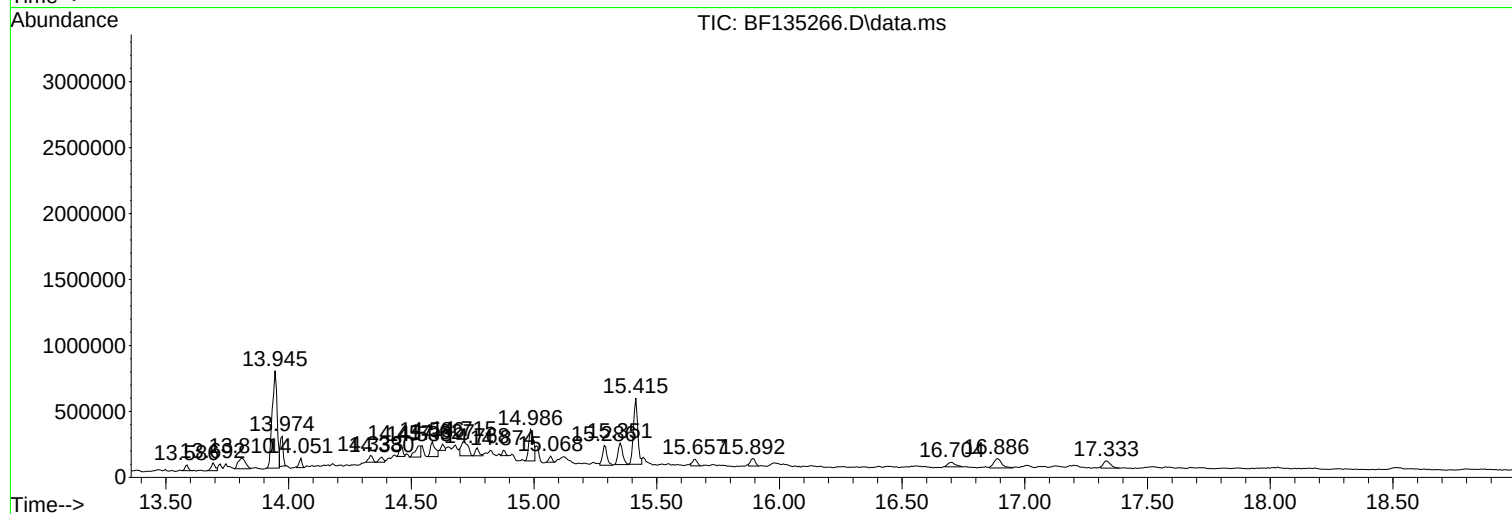
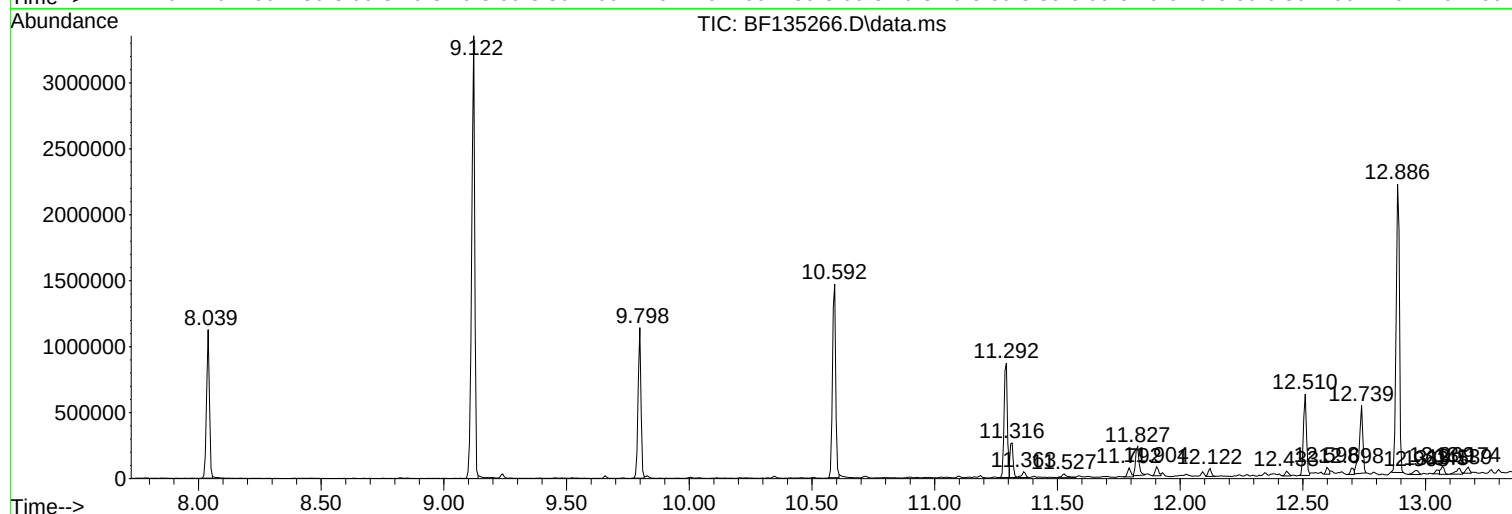
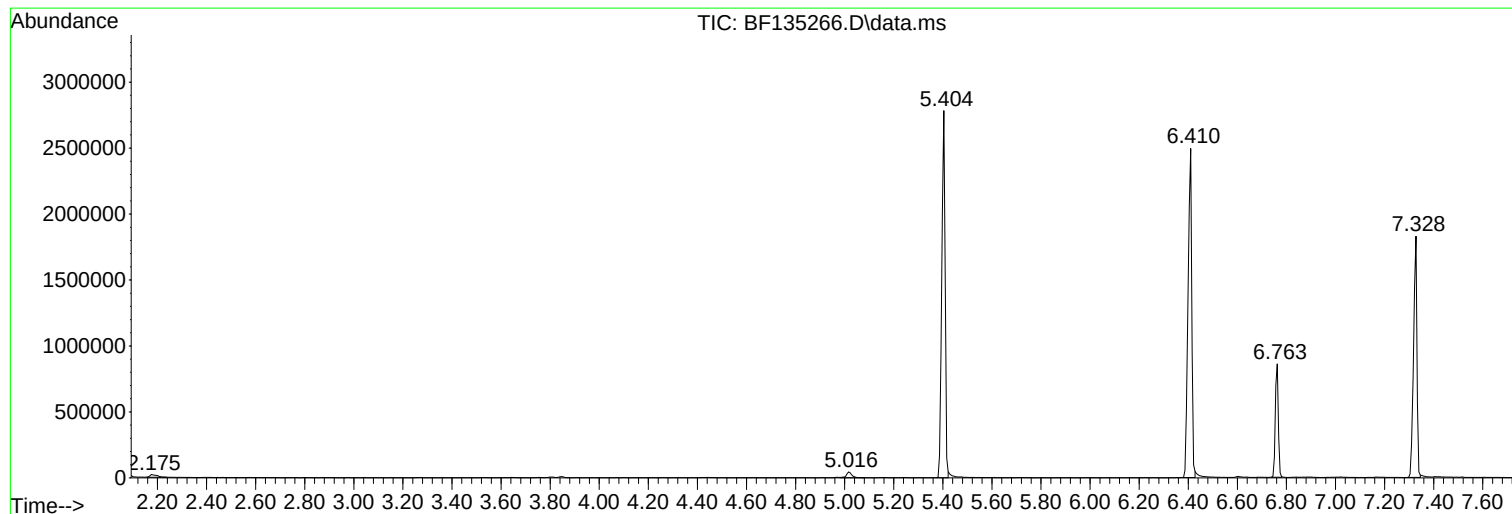
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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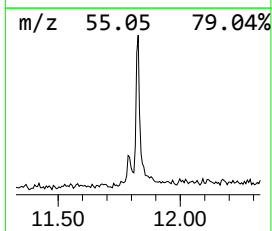
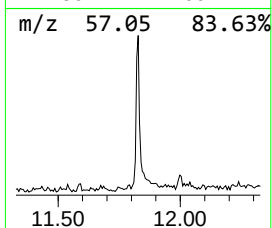
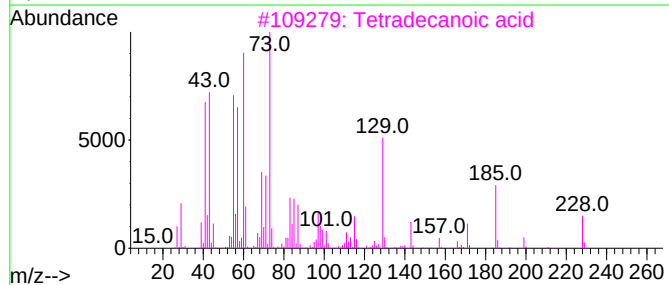
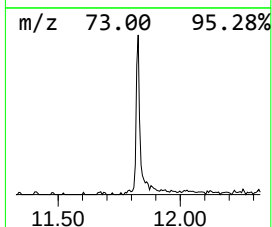
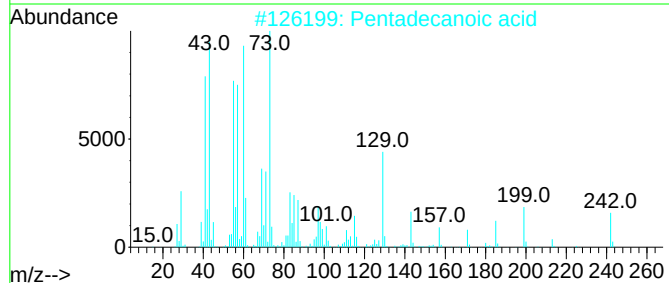
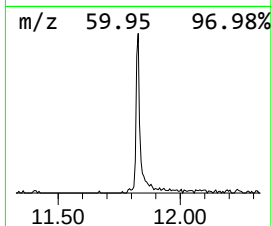
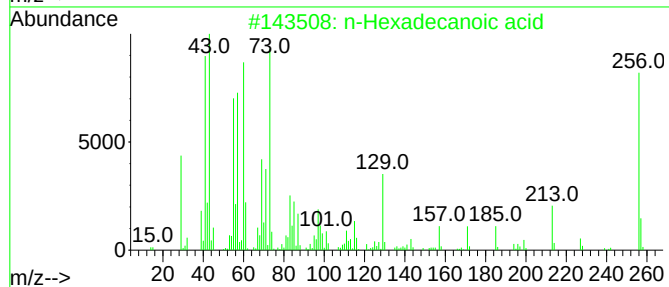
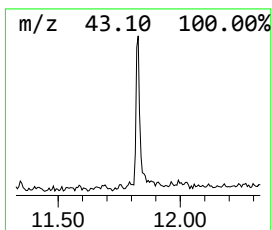
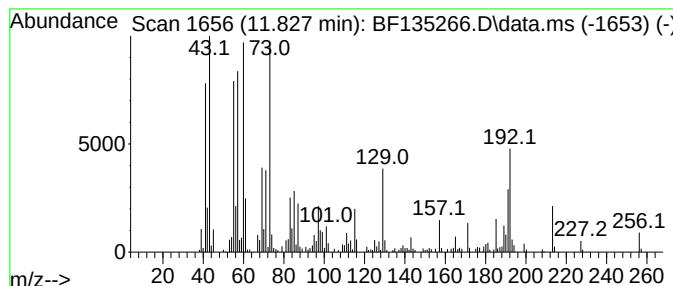
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.827	5.31 ng	217867	Phenanthrene-d10	11.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	62
4			Tridecanoic acid	214	C13H26O2	000638-53-9	60
5			Dodecanoic acid	200	C12H24O2	000143-07-7	52



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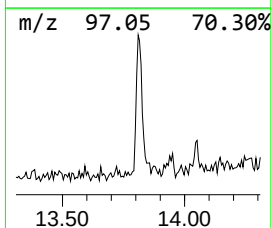
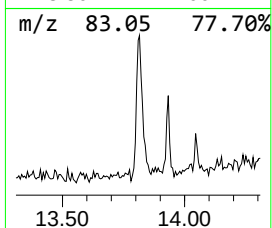
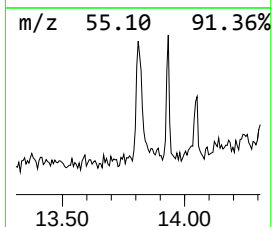
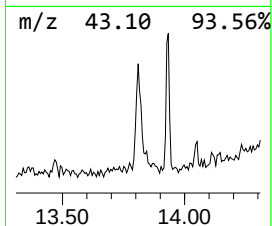
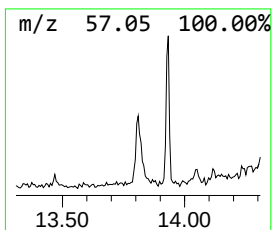
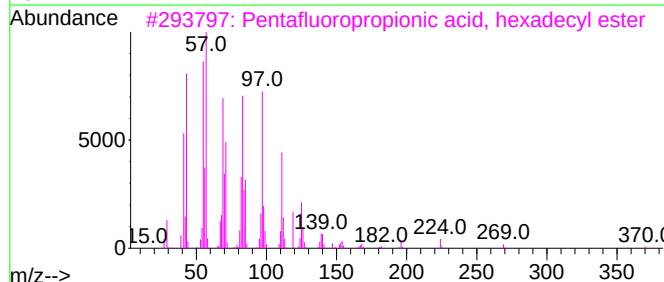
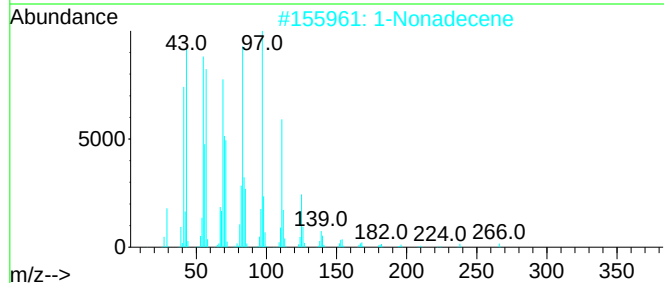
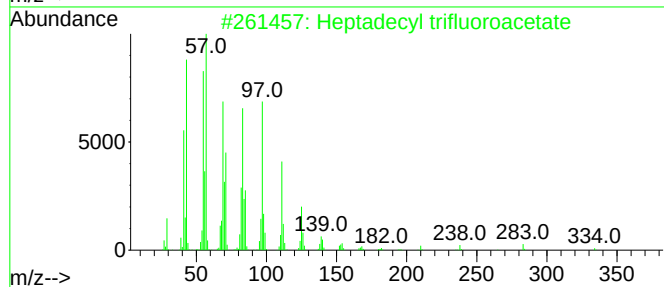
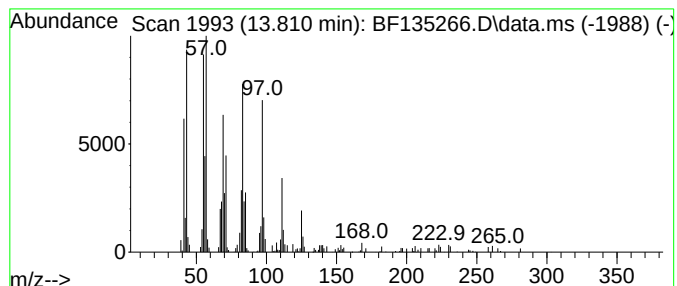
Instrument :
BNA_F
ClientSampleId :
72-11985

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 Heptadecyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.810	3.18 ng	165919	Chrysene-d12	13.945	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	Pentafluoropropionic acid, hexadecyl ester	388	C19H33F5O2	006222-07-7	91
4	Heptafluorobutyric acid, pentadecyl ester	424	C19H31F7O2	959261-23-5	91
5	11-Tricosene	322	C23H46	052078-56-5	91



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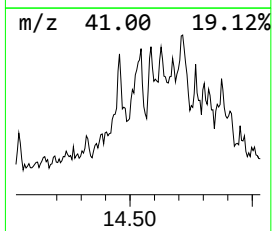
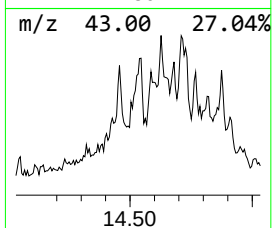
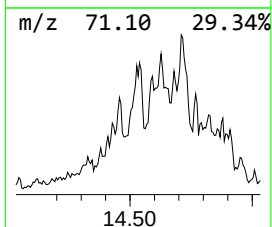
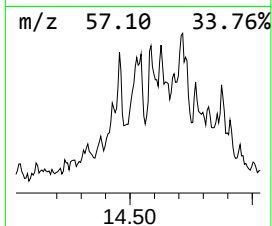
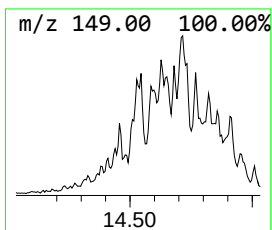
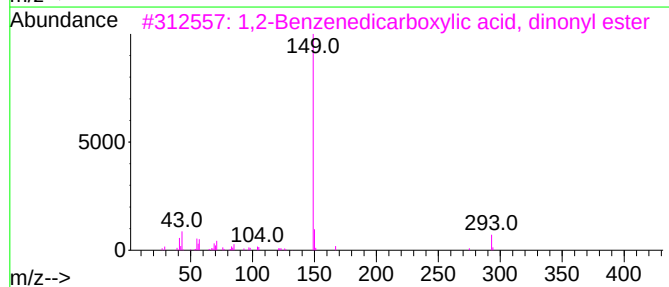
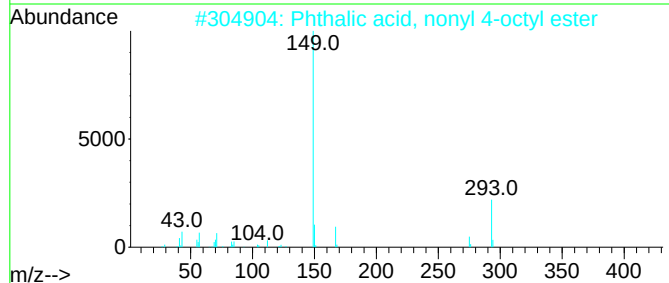
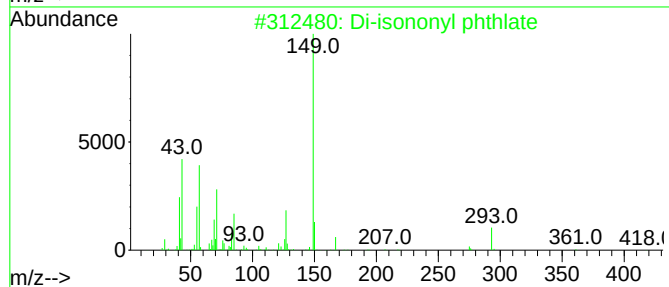
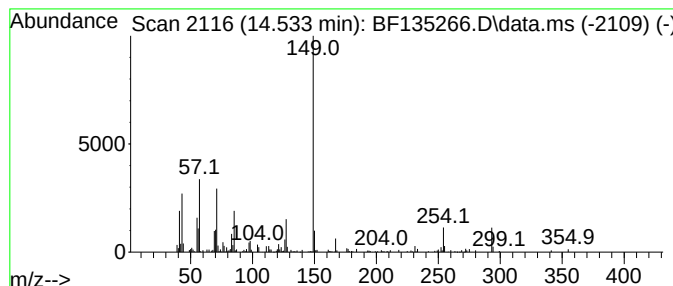
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Di-isnonyl phthlate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.533	2.81 ng	146221	Chrysene-d12	13.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-isnonyl phthlate	418	C26H42O4	020548-62-3	83
2			Phthalic acid, nonyl 4-octyl ester	404	C25H40O4	1000314-84-2	58
3			1,2-Benzenedicarboxylic acid, di...	418	C26H42O4	000084-76-4	53
4			Phthalic acid, cycloheptyl nonyl...	388	C24H36O4	1000322-83-4	50
5			Phthalic acid, isohexyl 5-methox...	364	C21H32O5	1000314-89-7	50



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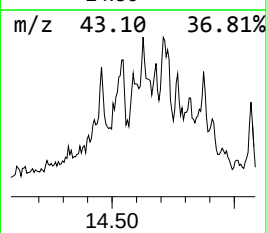
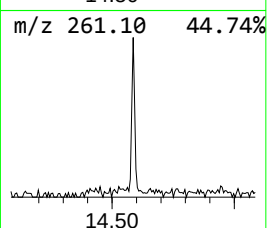
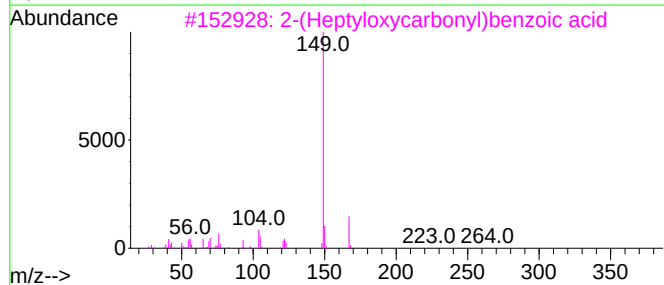
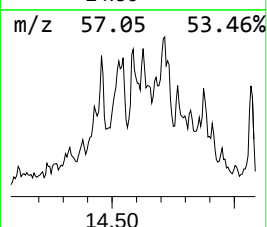
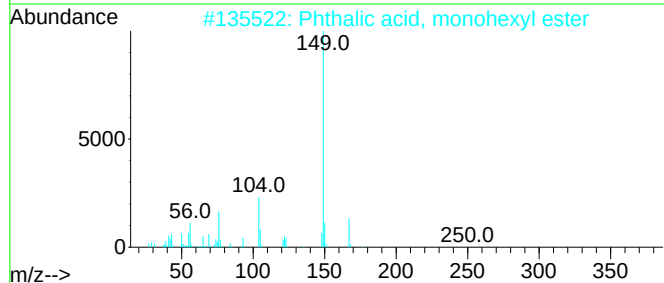
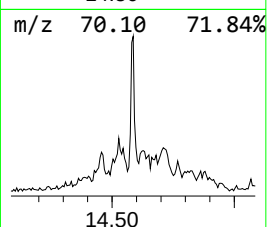
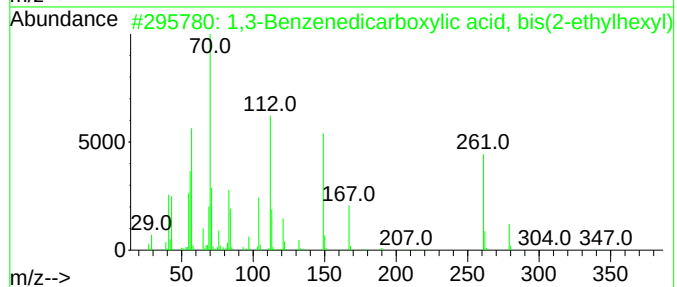
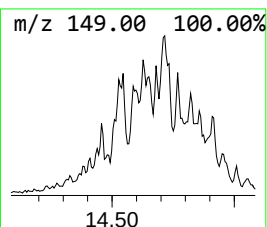
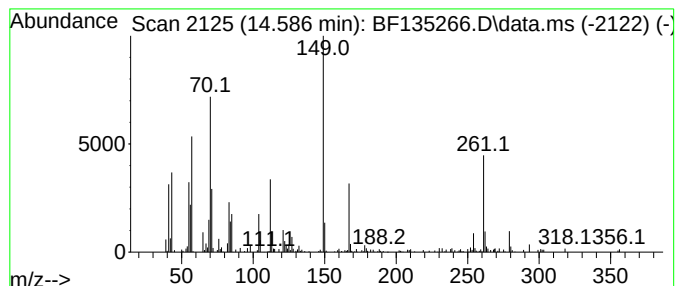
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown14.586 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.586	3.12 ng	162543	Chrysene-d12	13.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Benzenedicarboxylic acid, bi...	390	C24H3804	000137-89-3	46
2			Phthalic acid, monohexyl ester	250	C14H1804	024539-57-9	46
3			2-(Heptyloxycarbonyl)benzoic acid	264	C15H2004	024539-58-0	45
4			Bis(2-ethylhexyl) phthalate	390	C24H3804	000117-81-7	43
5			2-((2-Ethylbutoxy)carbonyl)benzo...	250	C14H1804	091401-46-6	38



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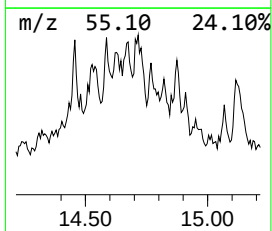
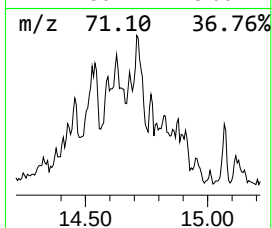
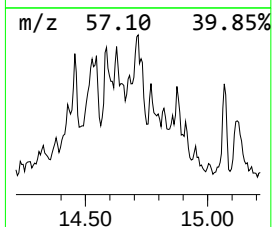
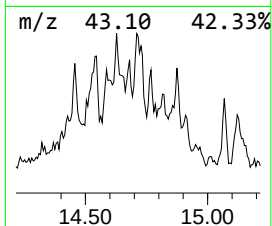
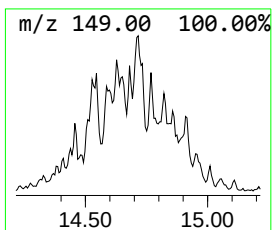
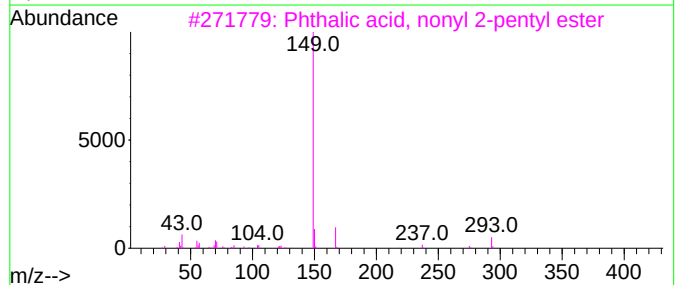
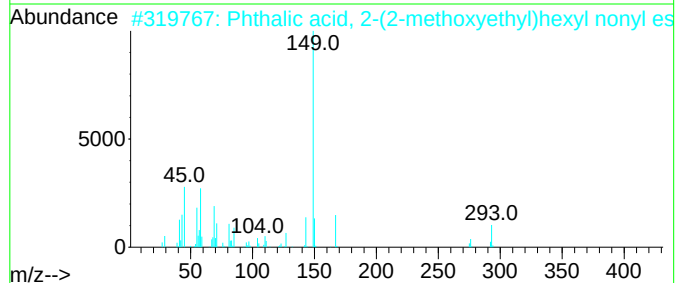
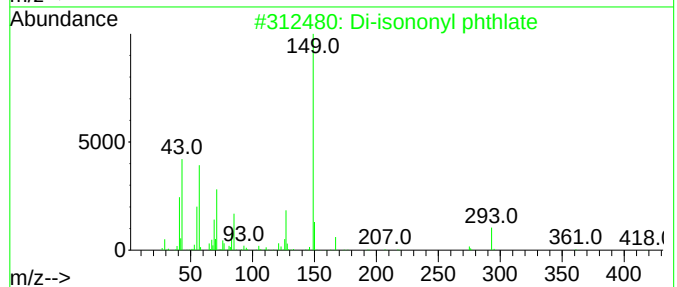
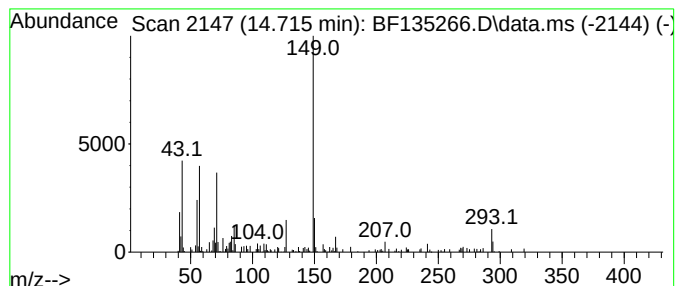
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Phthalic acid, 2-(2-methoxy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.716	6.66 ng	204889	Perylene-d12	15.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-isononyl phthlate	418	C26H42O4	020548-62-3	78
2			Phthalic acid, 2-(2-methoxyethyl...)	434	C26H42O5	1000314-93-3	59
3			Phthalic acid, nonyl 2-pentyl ester	362	C22H34O4	1000315-48-1	53
4			Phthalic acid, 2-ethylhexyl phen...	354	C22H26O4	1010315-51-4	53
5			1,2-Benzenedicarboxylic acid, de...	418	C26H42O4	000119-07-3	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091423\
Data File : BF135266.D
Acq On : 14 Sep 2023 21:42
Operator : CG\JU
Sample : 04399-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11985

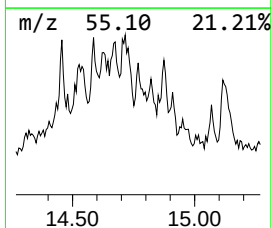
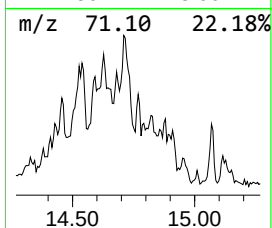
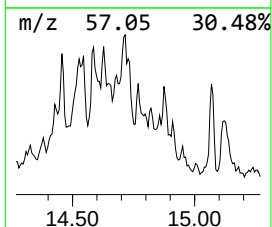
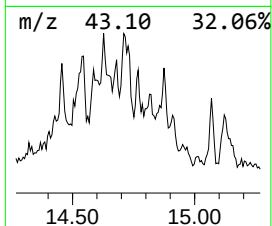
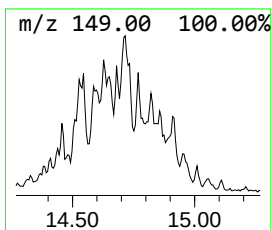
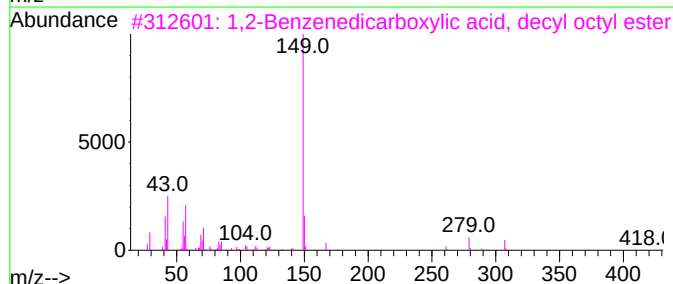
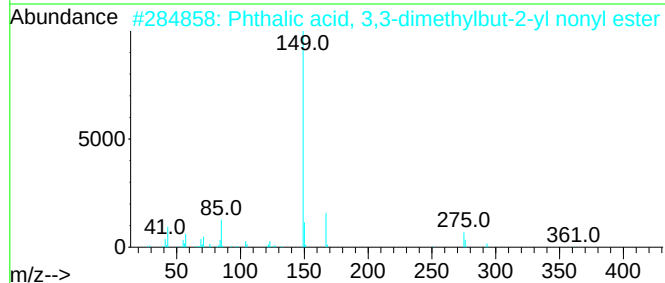
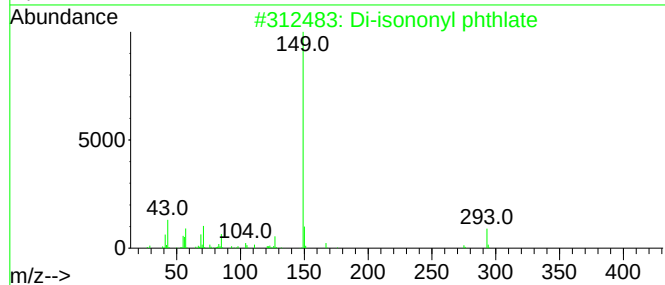
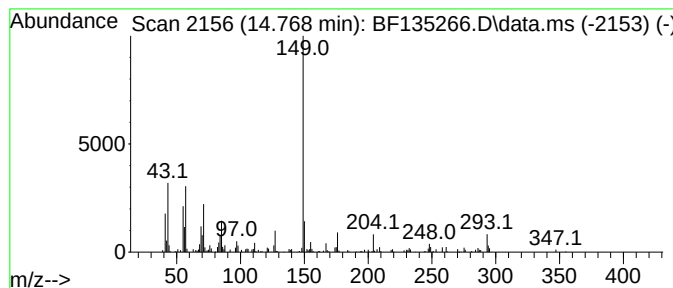
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Phthalic acid, 3,3-dimethyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.768	2.13 ng	65587	Perylene-d12	15.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-isononyl phthlate	418	C26H42O4	020548-62-3	59
2			Phthalic acid, 3,3-dimethylbut-2...	376	C23H36O4	1000357-00-8	53
3			1,2-Benzenedicarboxylic acid, de...	418	C26H42O4	000119-07-3	50
4			Phthalic acid, hept-2-yl nonyl e...	390	C24H38O4	1000356-97-6	50
5			Phthalic acid, 2-ethylhexyl phen...	354	C22H26O4	1010315-51-4	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091423\
Data File : BF135266.D
Acq On : 14 Sep 2023 21:42
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Sample : 04399-03
Misc :
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Instrument :
BNA_F
ClientSampleId :
72-11985

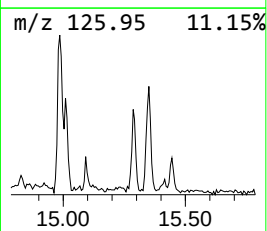
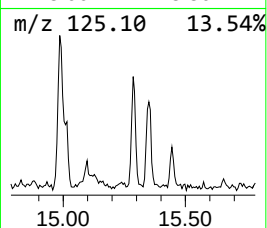
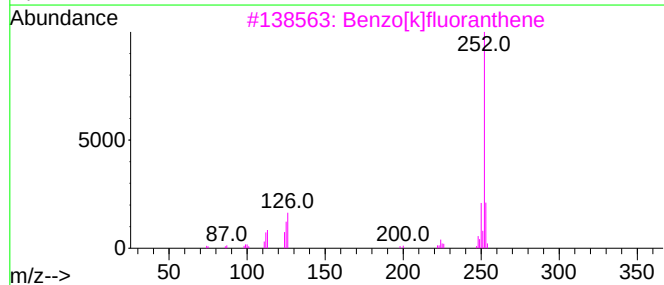
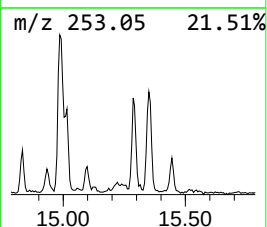
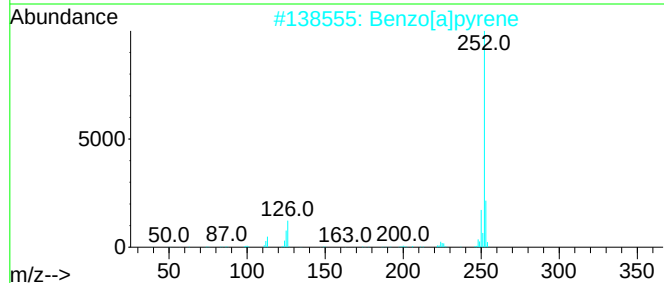
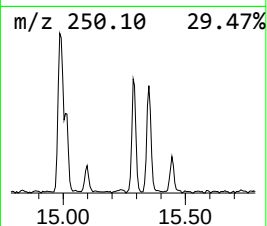
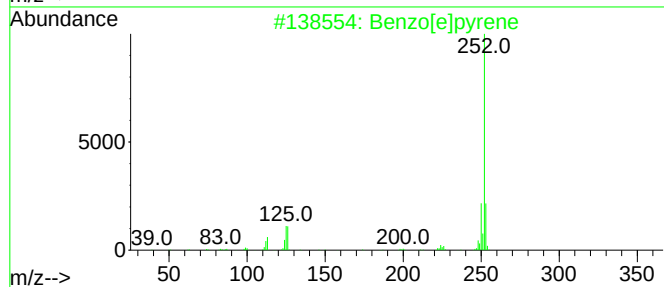
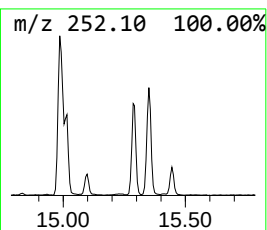
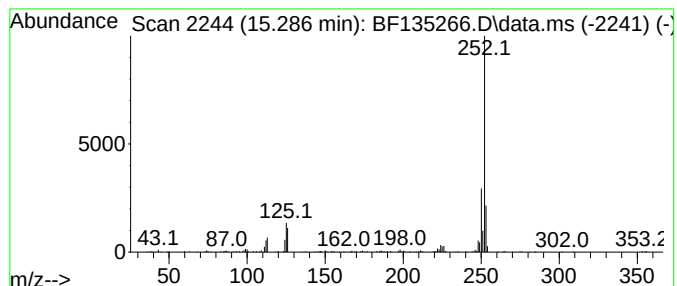
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.286	6.08 ng	187063	Perylene-d12	15.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Benzo[a]pyrene	252	C20H12	000050-32-8	96
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
5			Perylene	252	C20H12	000198-55-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091423\
Data File : BF135266.D
Acq On : 14 Sep 2023 21:42
Operator : CG\JU
Sample : 04399-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

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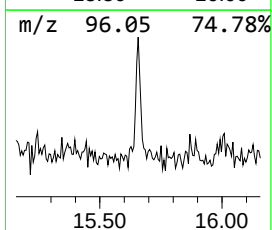
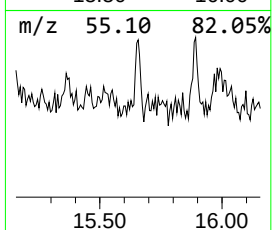
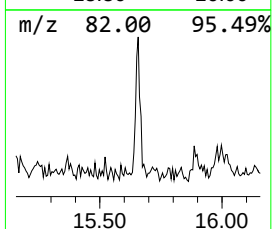
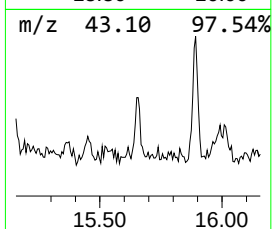
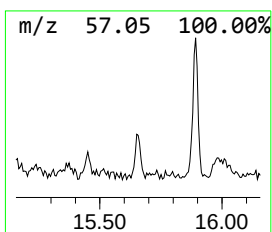
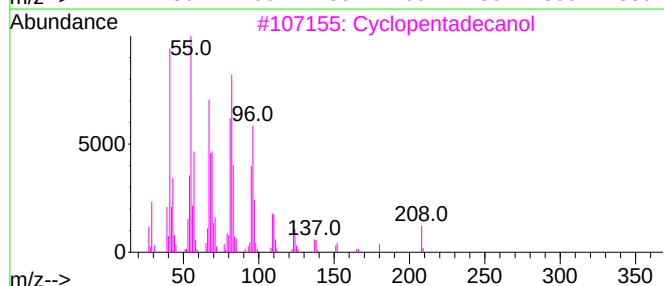
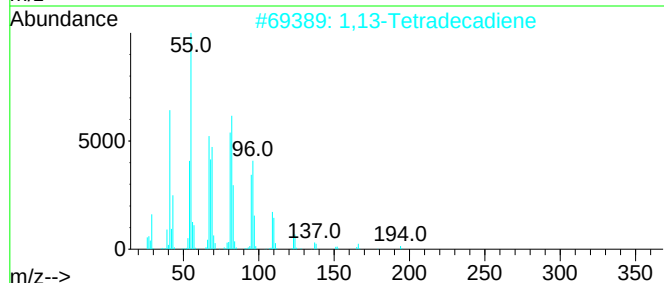
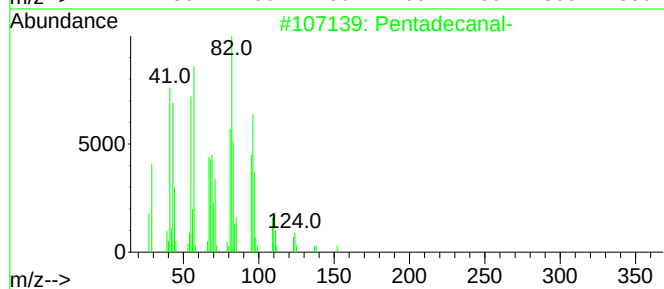
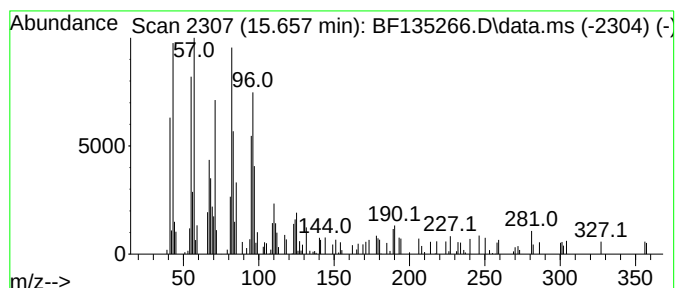
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentadecanal- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.657	2.11 ng	64898	Perylene-d12	15.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanal-	226	C15H30O	002765-11-9	62
2			1,13-Tetradecadiene	194	C14H26	021964-49-8	60
3			Cyclopentadecanol	226	C15H30O	004727-17-7	58
4			9-Octadecen-1-ol, (Z)-	268	C18H36O	000143-28-2	58
5			Hexadecanal	240	C16H32O	000629-80-1	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091423\
Data File : BF135266.D
Acq On : 14 Sep 2023 21:42
Operator : CG\JU
Sample : 04399-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

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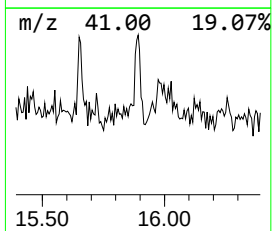
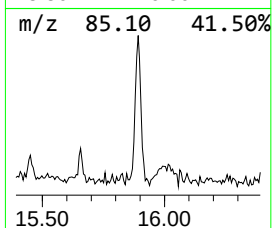
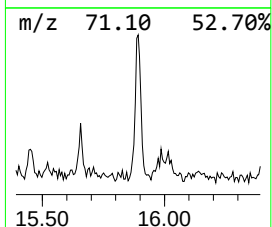
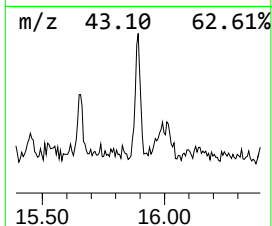
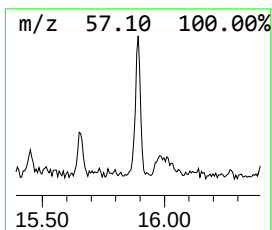
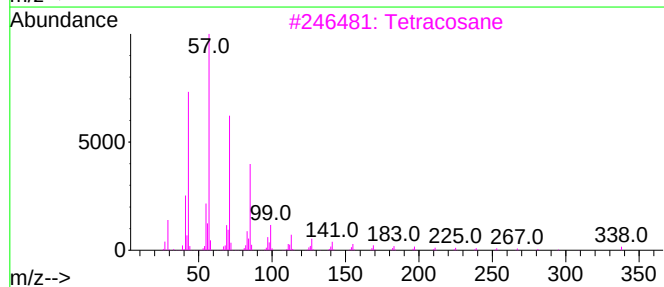
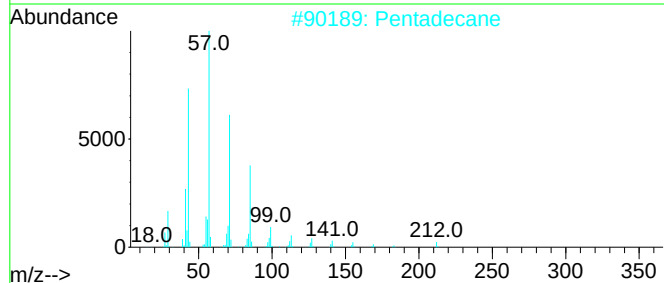
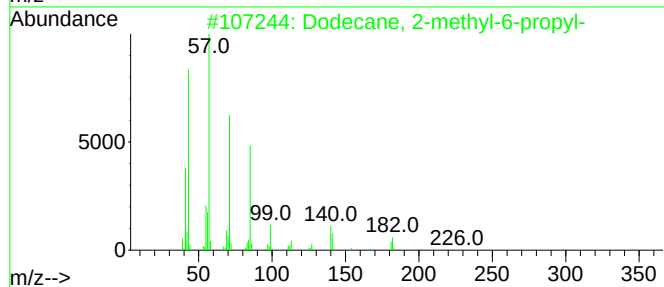
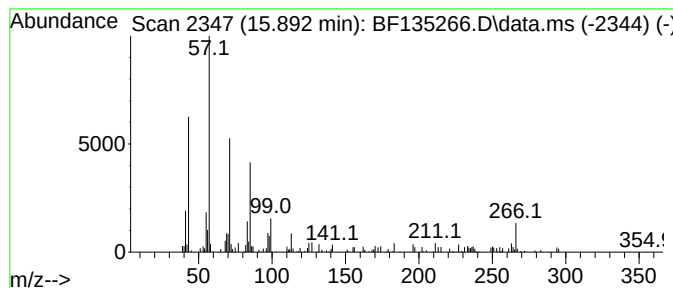
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Dodecane, 2-methyl-6-propyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.892	2.51 ng	77208	Perylene-d12	15.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	74
2			Pentadecane	212	C15H32	000629-62-9	74
3			Tetracosane	338	C24H50	000646-31-1	74
4			Nonadecane	268	C19H40	000629-92-5	72
5			Hexadecane	226	C16H34	000544-76-3	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091423\
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Acq On : 14 Sep 2023 21:42
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Sample : 04399-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

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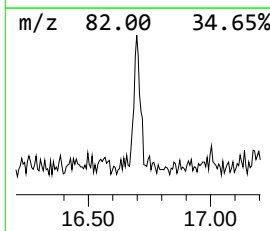
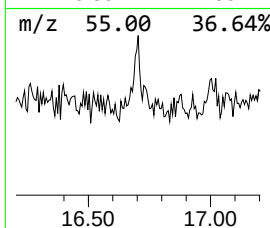
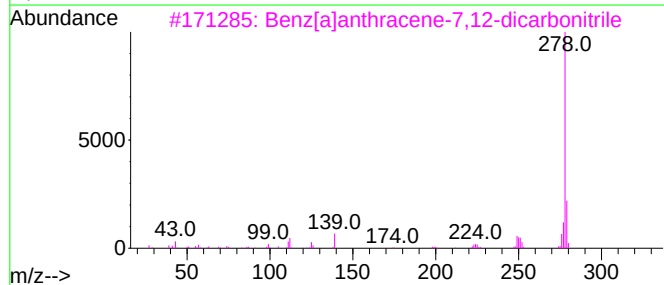
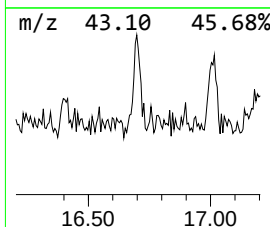
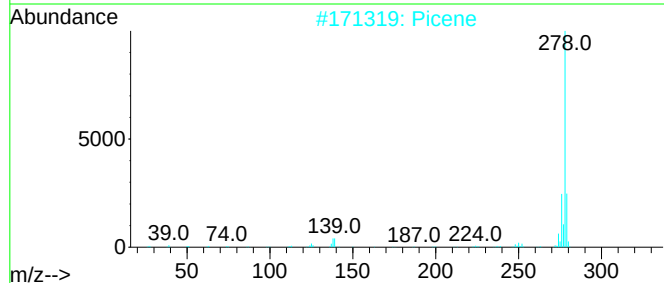
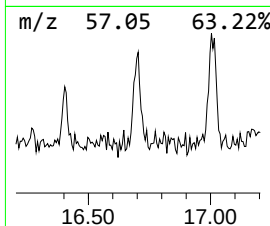
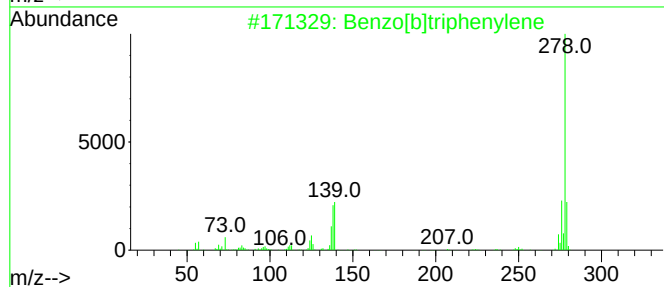
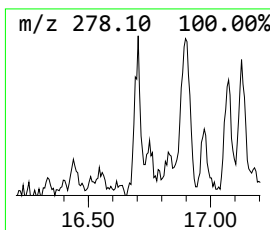
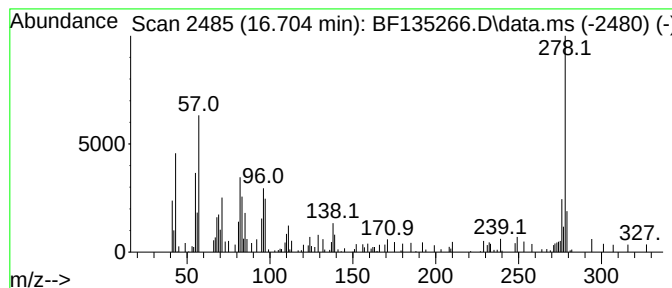
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzo[b]triphenylene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.704	2.46 ng	75665	Perylene-d12	15.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]triphenylene	278	C22H14	000215-58-7	53
2			Picene	278	C22H14	000213-46-7	46
3			Benz[a]anthracene-7,12-dicarboni...	278	C20H10N2	035215-32-8	46
4			Estra-1,3,5,7,9,15-hexaen-17-one...	278	C19H18O2	056588-53-5	43
5			Pyridine-3-carbonitrile, 2-oxo-4...	278	C16H10N2O5	1000304-72-3	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091423\
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Acq On : 14 Sep 2023 21:42
Operator : CG\JU
Sample : 04399-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

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ClientSampleId :
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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
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Heptadecyl trif...	13.810	3.2	ng	165919	5	13.945	1042080	20.0
Di-isononyl pht...	14.533	2.8	ng	146221	5	13.945	1042080	20.0
unknown14.586	14.586	3.1	ng	162543	5	13.945	1042080	20.0
Phthalic acid, ...	14.716	6.7	ng	204889	6	15.415	614927	20.0
Phthalic acid, ...	14.768	2.1	ng	65587	6	15.415	614927	20.0
Benzo[e]pyrene	15.286	6.1	ng	187063	6	15.415	614927	20.0
Pentadecanal-	15.657	2.1	ng	64898	6	15.415	614927	20.0
Dodecane, 2-met...	15.892	2.5	ng	77208	6	15.415	614927	20.0
Benzo[b]triphen...	16.704	2.5	ng	75665	6	15.415	614927	20.0