

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071123\
 Data File : BF134236.D
 Acq On : 12 Jul 2023 03:54
 Operator : CG\JU
 Sample : 03375-07 5X
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-3(0-2)

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-BF062623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134236.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.069	501	507	513	rBV	14672	18709	1.69%	0.219%
2	5.475	573	576	585	rBV	354750	354890	32.10%	4.148%
3	6.481	744	747	759	rBV	344746	352717	31.90%	4.122%
4	6.845	805	809	815	rBV	677888	539911	48.83%	6.310%
5	7.404	901	904	912	rBV	221312	200363	18.12%	2.342%
6	8.128	1023	1027	1030	rBV	666468	607674	54.96%	7.102%
7	9.198	1206	1209	1218	rBV	408415	333954	30.21%	3.903%
8	9.886	1322	1326	1329	rBV	571680	526080	47.58%	6.149%
9	10.598	1444	1447	1451	rBV2	31736	26563	2.40%	0.310%
10	10.675	1457	1460	1469	rBV	204454	189092	17.10%	2.210%
11	11.186	1544	1547	1550	rBV	31228	28671	2.59%	0.335%
12	11.275	1560	1562	1568	rVB	12771	12917	1.17%	0.151%
13	11.380	1576	1580	1582	rBV	619839	522735	47.28%	6.110%
14	11.404	1582	1584	1588	rVB	292657	221307	20.02%	2.587%
15	11.480	1595	1597	1605	rVB7	8061	12350	1.12%	0.144%
16	11.616	1616	1620	1625	rBV	25773	33646	3.04%	0.393%
17	11.886	1662	1666	1667	rBV	29998	28579	2.58%	0.334%
18	11.910	1667	1670	1674	rVV2	128008	151870	13.74%	1.775%
19	11.945	1674	1676	1681	rVV	52739	52655	4.76%	0.615%
20	11.992	1681	1684	1687	rVV2	28743	35165	3.18%	0.411%
21	12.022	1687	1689	1694	rVB	19463	18396	1.66%	0.215%
22	12.180	1714	1716	1719	rBV	28793	26045	2.36%	0.304%
23	12.210	1719	1721	1726	rVB	89480	78789	7.13%	0.921%
24	12.439	1757	1760	1761	rBV2	19670	19474	1.76%	0.228%
25	12.457	1761	1763	1768	rVB4	20667	29918	2.71%	0.350%
26	12.527	1772	1775	1780	rVB	48668	51528	4.66%	0.602%
27	12.604	1784	1788	1791	rBV	475120	414020	37.45%	4.839%
28	12.698	1801	1804	1808	rBV2	48347	52995	4.79%	0.619%
29	12.833	1821	1827	1833	rBV	360610	380587	34.42%	4.448%
30	12.880	1833	1835	1837	rVV3	19983	13916	1.26%	0.163%
31	12.974	1845	1851	1859	rBV	337936	352000	31.84%	4.114%
32	13.051	1861	1864	1868	rVV3	21868	35653	3.22%	0.417%
33	13.139	1877	1879	1880	rBV2	19631	16189	1.46%	0.189%
34	13.269	1896	1901	1904	rBV3	33193	57043	5.16%	0.667%
35	13.363	1914	1917	1920	rBV3	29097	27151	2.46%	0.317%
36	13.392	1920	1922	1925	rBV3	19915	21407	1.94%	0.250%

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Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

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-BF062623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.457	1929	1933	1936	rBV	294521	255308	23.09%	2.984%
38	13.680	1968	1971	1976	rBV	69476	77410	7.00%	0.905%
39	13.786	1987	1989	1992	rBV	40213	36418	3.29%	0.426%
40	13.845	1996	1999	2000	rBV	31696	35364	3.20%	0.413%
41	13.886	2004	2006	2009	rVV	50675	48776	4.41%	0.570%
42	14.016	2025	2028	2031	rBV	1051048	1105611	100.00%	12.922%
43	14.039	2031	2032	2035	rVV	478296	428841	38.79%	5.012%
44	14.069	2035	2037	2042	rVB	176078	154509	13.97%	1.806%
45	14.174	2052	2055	2056	rBV	54208	52372	4.74%	0.612%
46	15.110	2210	2214	2217	rBV	118582	182355	16.49%	2.131%
47	15.551	2285	2289	2298	rVB	249947	334130	30.22%	3.905%

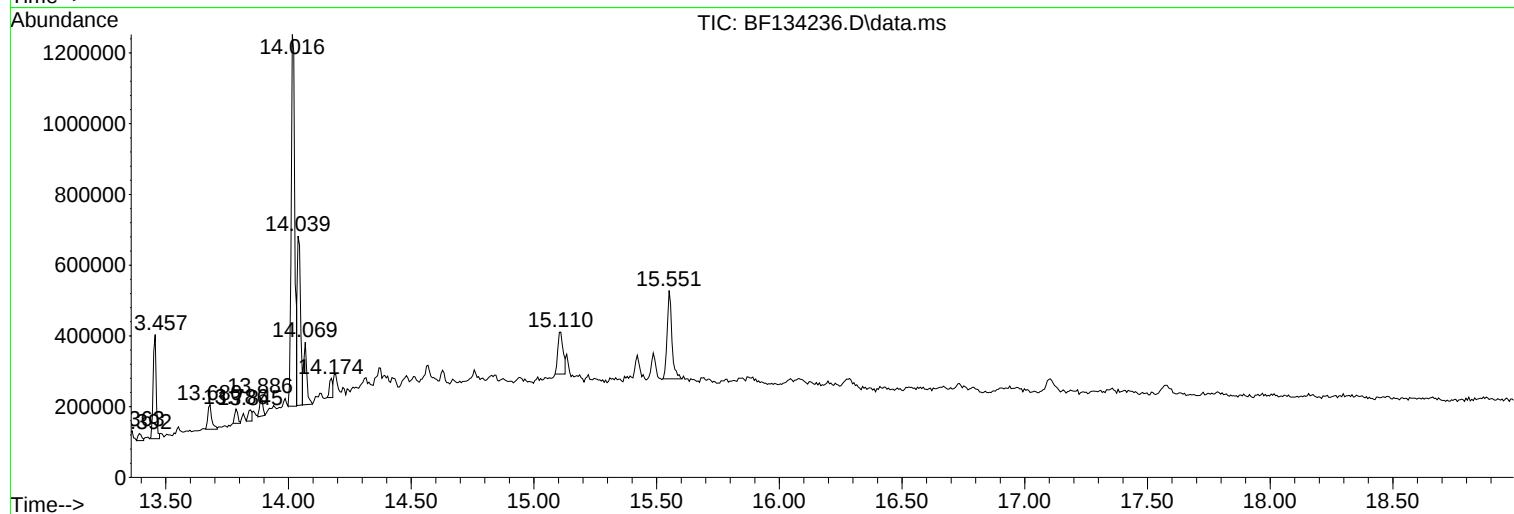
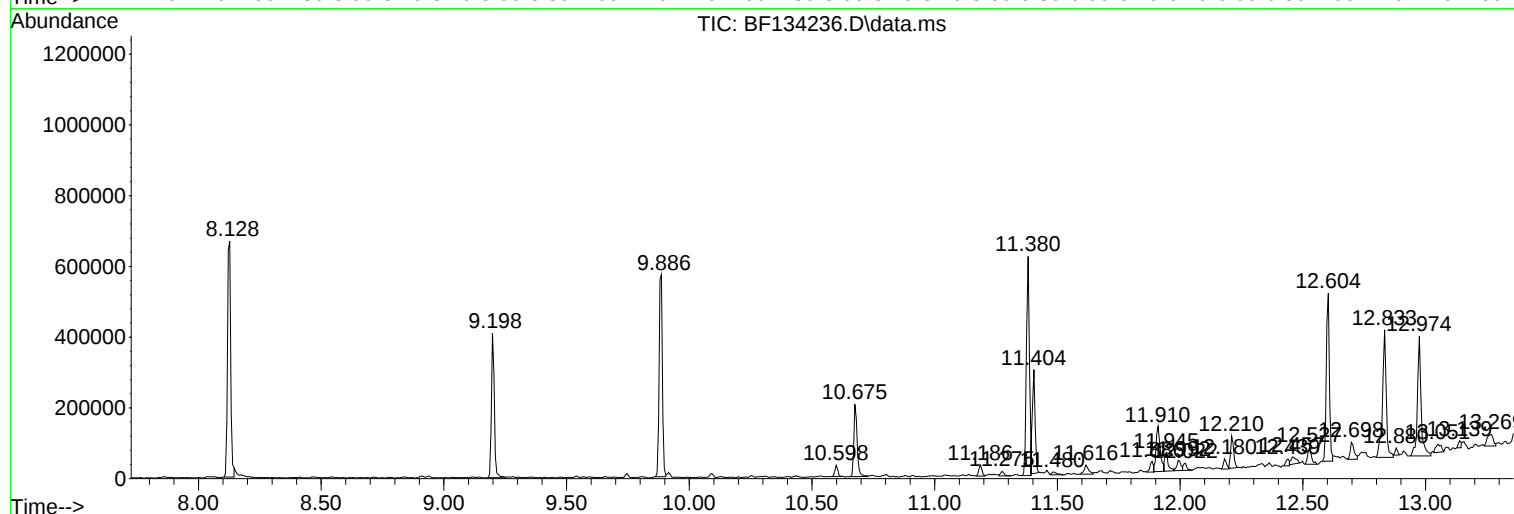
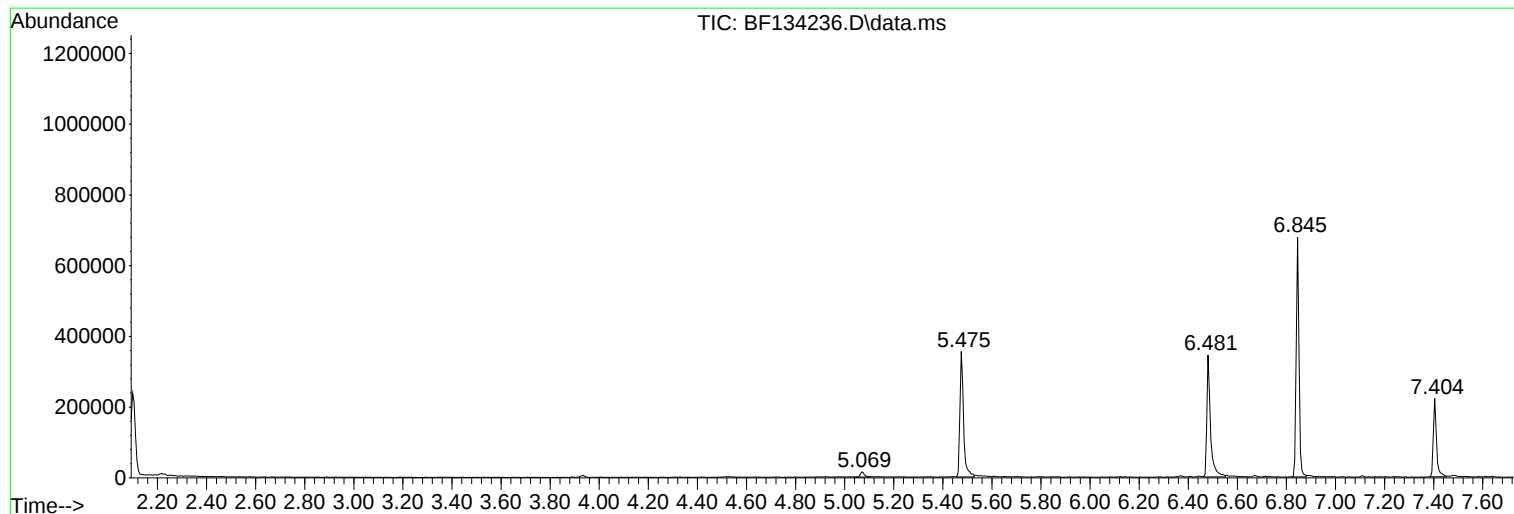
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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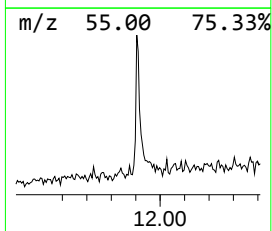
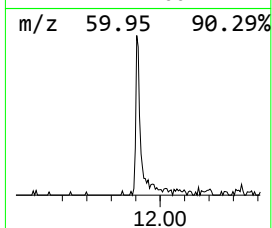
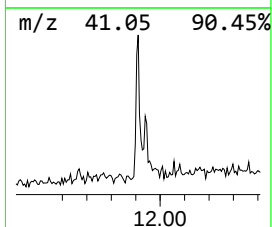
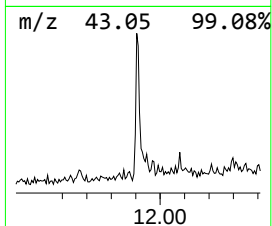
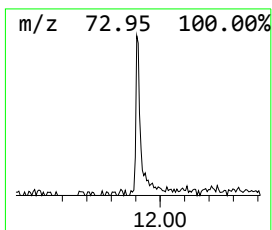
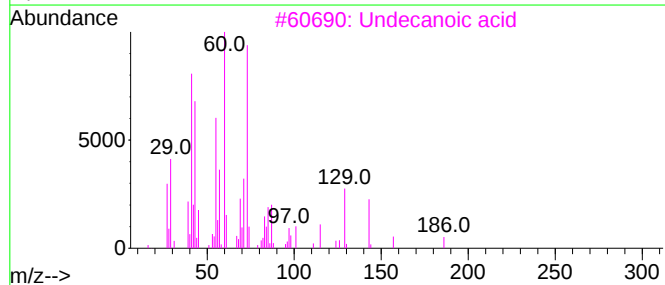
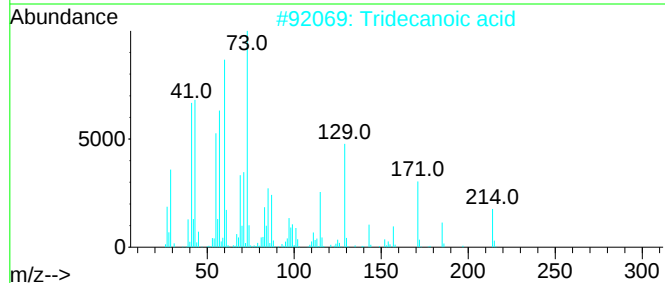
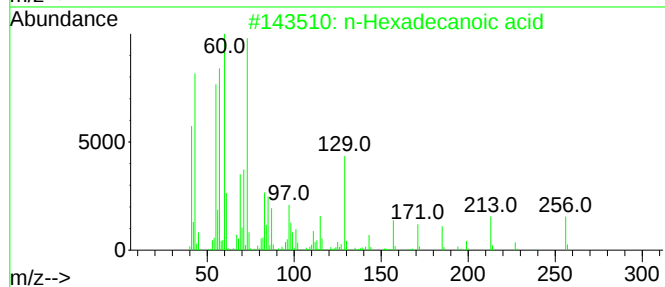
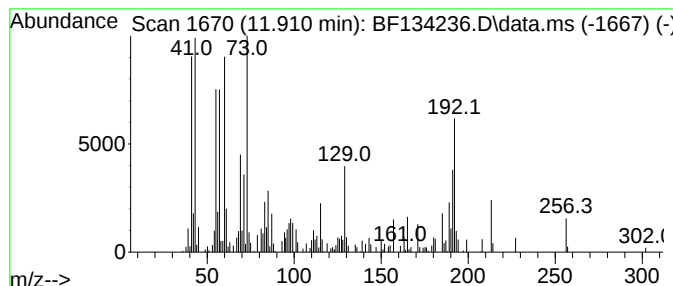
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	5.81 ng	151870	Phenanthrene-d10	11.380

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
2		Tridecanoic acid	214	C13H26O2	000638-53-9	91
3		Undecanoic acid	186	C11H22O2	000112-37-8	60
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5		n-Decanoic acid	172	C10H20O2	000334-48-5	50



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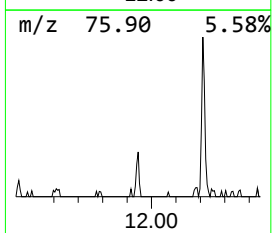
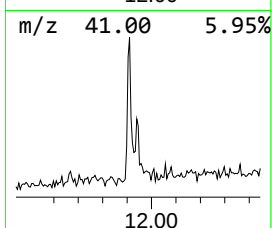
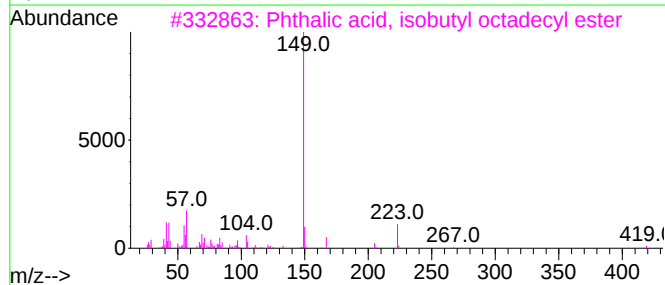
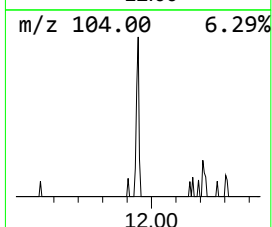
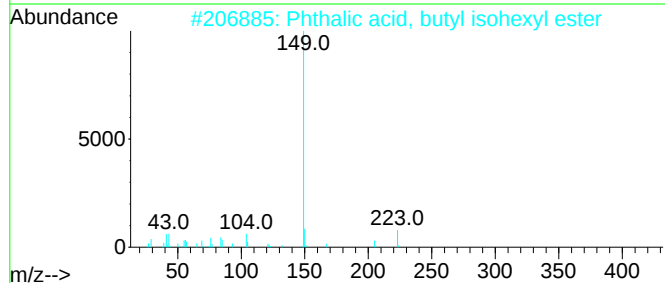
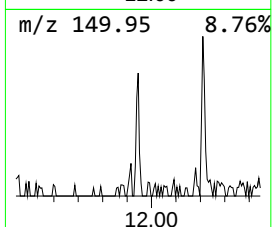
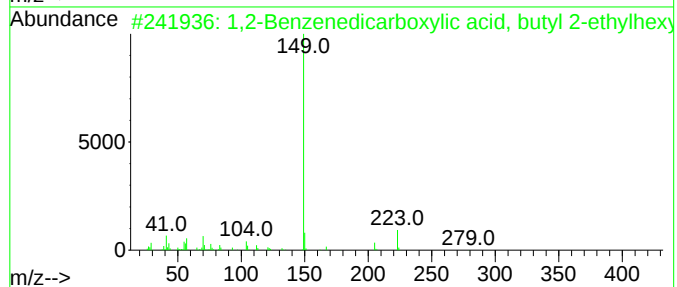
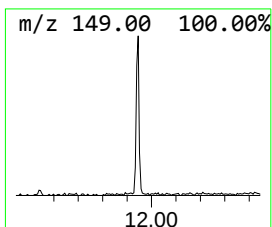
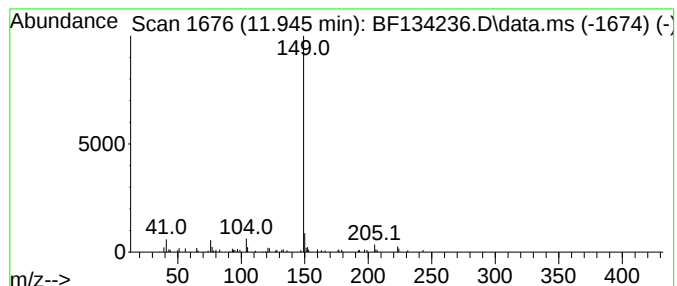
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 1,2-Benzenedicarboxylic aci... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	2.01 ng	52655	Phenanthrene-d10	11.380

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000085-69-8	78
2			Phthalic acid, butyl isohexyl ester	306	C18H26O4	1000309-03-6	78
3			Phthalic acid, isobutyl octadecy...	474	C30H50O4	1000309-06-1	78
4			1,4-Dibutyl benzene-1,4-dicarbox...	278	C16H22O4	001962-75-0	72
5			Phthalic acid, isobutyl cyclohex...	318	C19H26O4	1000308-94-3	72



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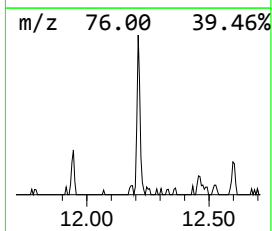
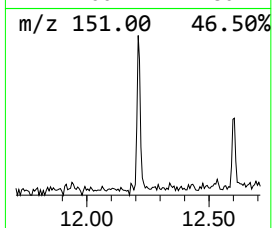
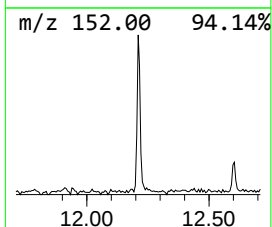
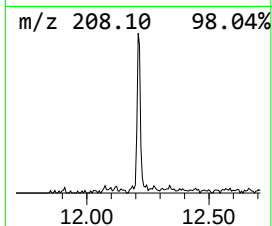
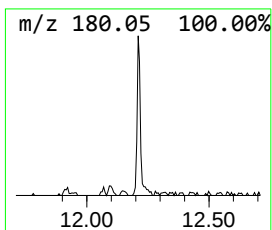
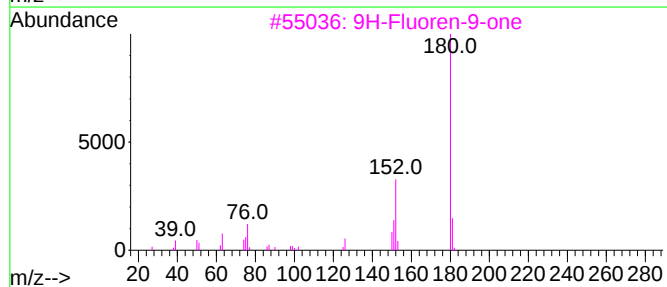
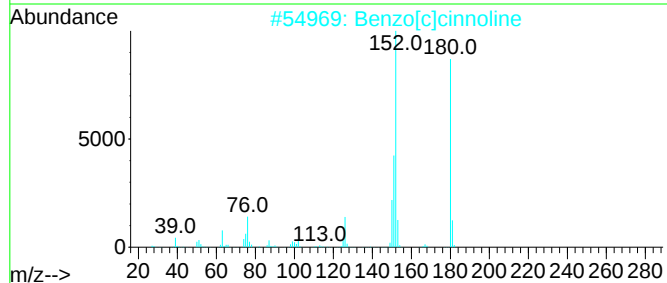
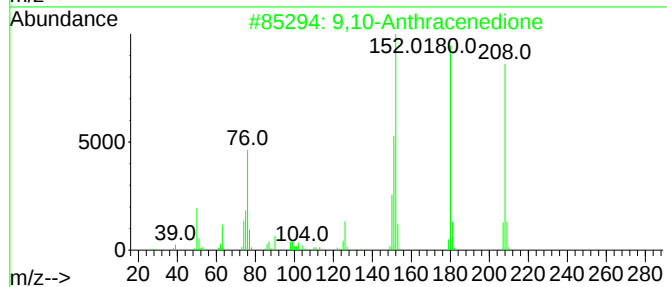
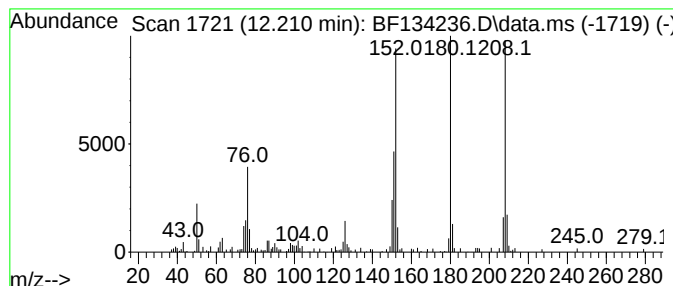
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 9,10-Anthracenedione Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.210	3.01 ng	78789	Phenanthrene-d10	11.380

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9,10-Anthracenedione	208	C14H8O2	000084-65-1	99
2		Benzo[c]cinnoline	180	C12H8N2	000230-17-1	93
3		9H-Fluoren-9-one	180	C13H8O	000486-25-9	91
4		1H-Phenalen-1-one	180	C13H8O	000548-39-0	60
5		Benzo[h]cinnoline	180	C12H8N2	000230-31-9	60



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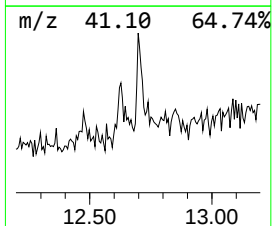
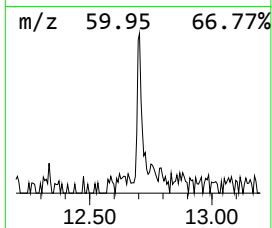
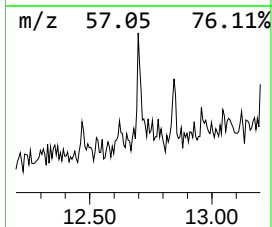
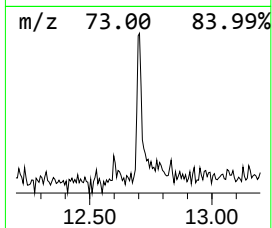
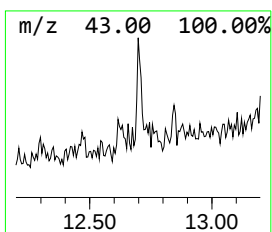
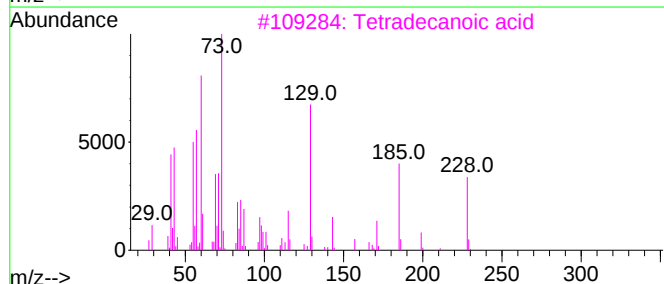
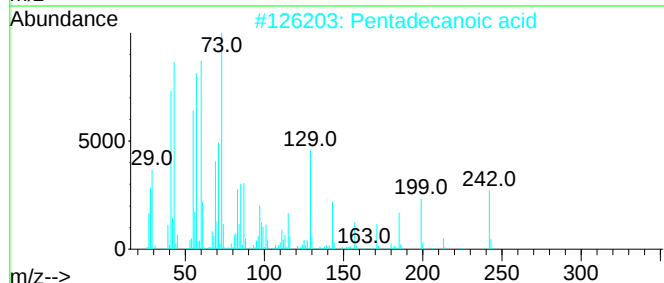
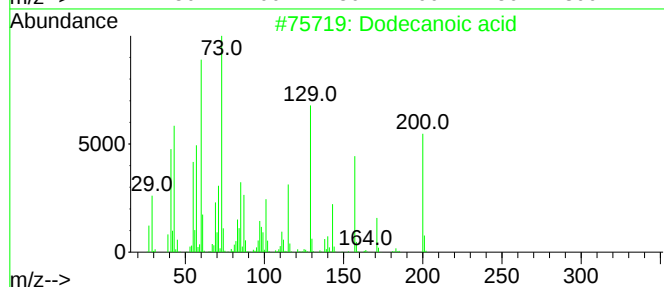
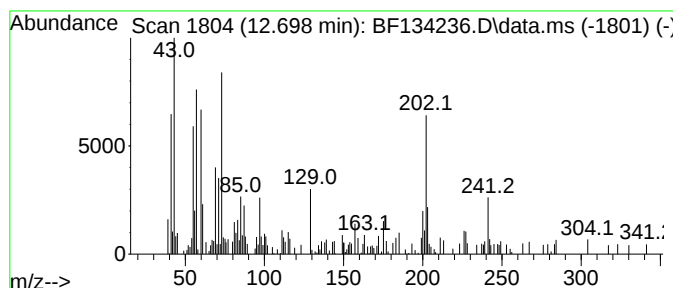
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown12.698 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.698	2.03 ng	52995	Phenanthrene-d10		11.380	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Dodecanoic acid		200	C12H24O2	000143-07-7	43
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	43
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	42
4	n-Decanoic acid		172	C10H20O2	000334-48-5	38
5	8-Methylnonanoic acid		172	C10H20O2	005963-14-4	35



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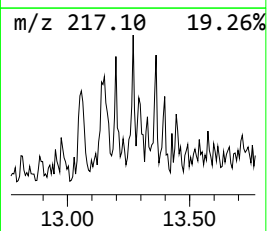
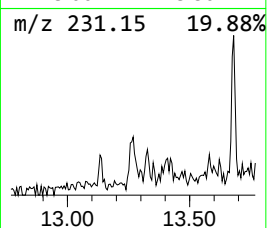
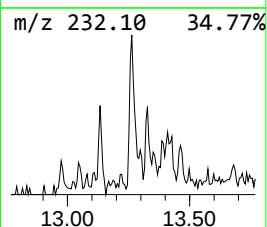
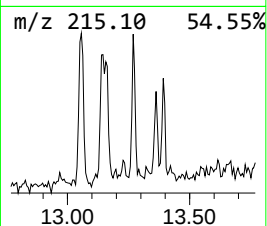
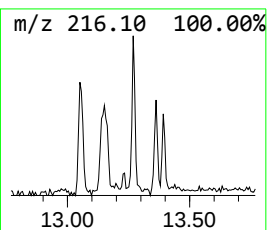
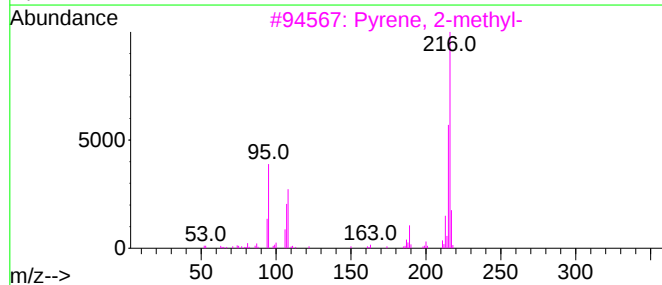
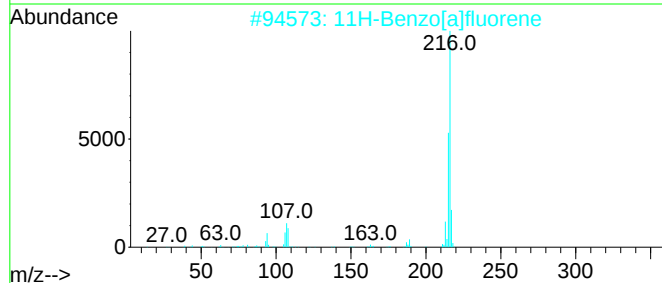
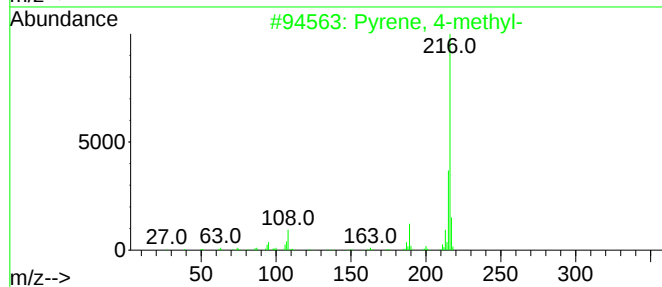
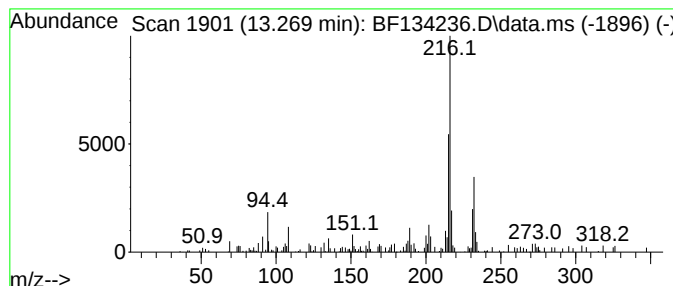
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pyrene, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.269	2.66 ng	57043	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene, 4-methyl-	216	C17H12	003353-12-6	78
2			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	64
3			Pyrene, 2-methyl-	216	C17H12	003442-78-2	64
4			Pyrene, 1-methyl-	216	C17H12	002381-21-7	64
5			Allopregnane-3.alpha.,20.alpha.-...	320	C21H36O2	000566-58-5	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071123\
Data File : BF134236.D
Acq On : 12 Jul 2023 03:54
Operator : CG\JU
Sample : 03375-07 5X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3(0-2)

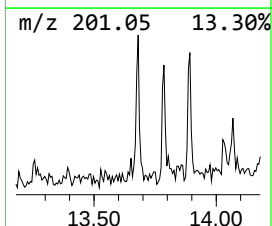
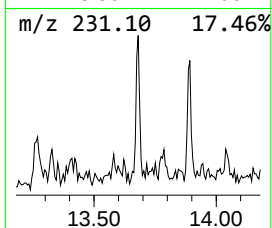
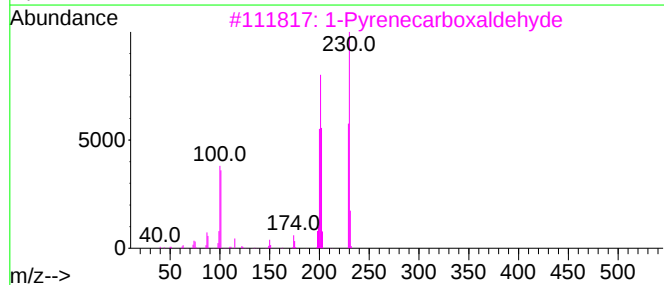
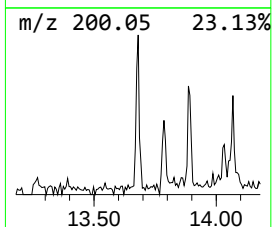
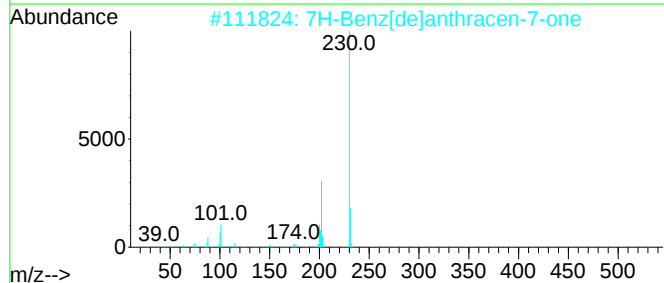
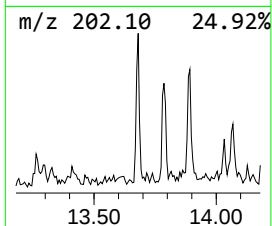
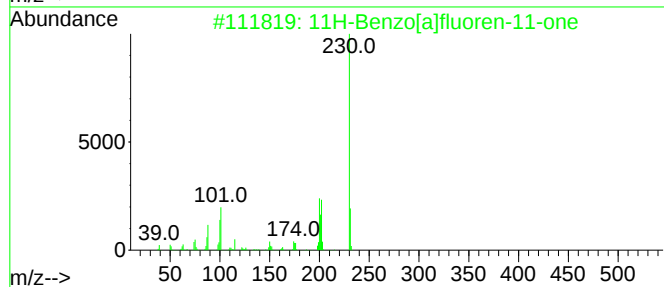
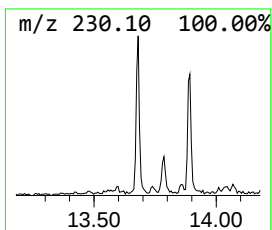
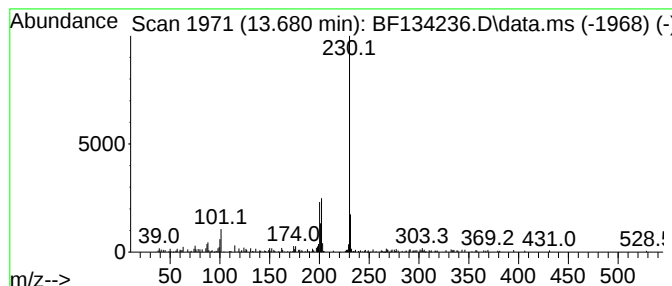
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 11H-Benzo[a]fluoren-11-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.680	3.61 ng	77410	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	93
2			7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	93
3			1-Pyrenecarboxaldehyde	230	C17H10O	003029-19-4	80
4			4-Pyrenecarbaldehyde	230	C17H10O	022245-51-8	72
5			6H-Benz[de]anthracen-6-one	230	C17H10O	080252-14-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071123\
Data File : BF134236.D
Acq On : 12 Jul 2023 03:54
Operator : CG\JU
Sample : 03375-07 5X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3(0-2)

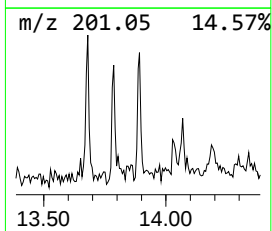
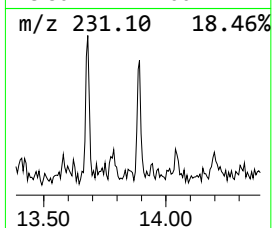
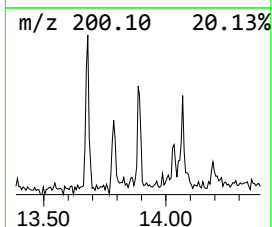
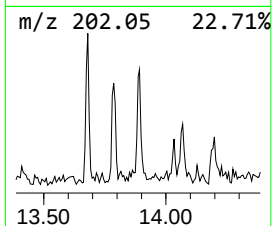
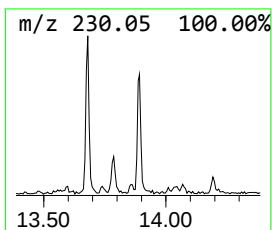
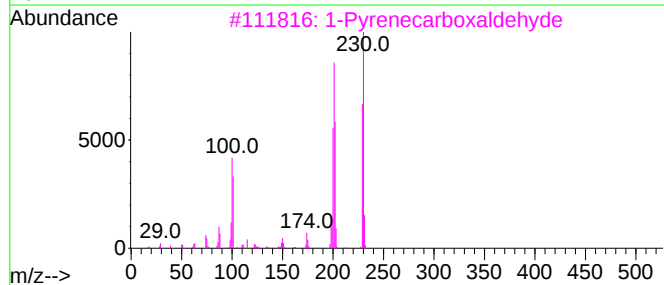
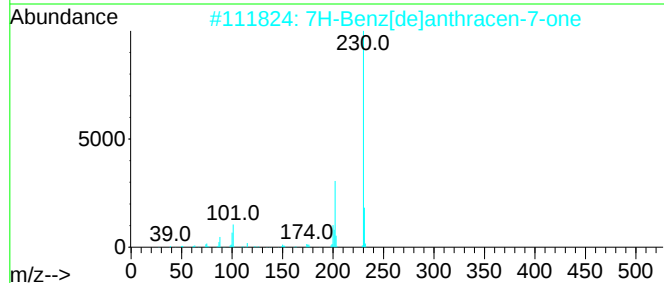
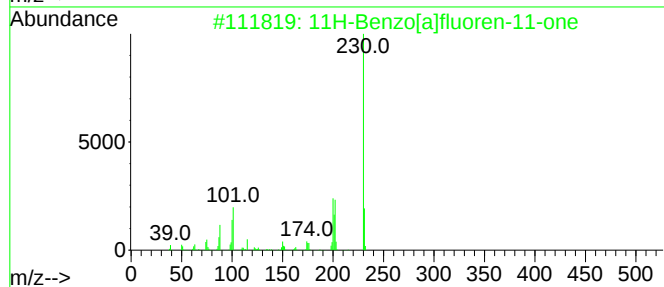
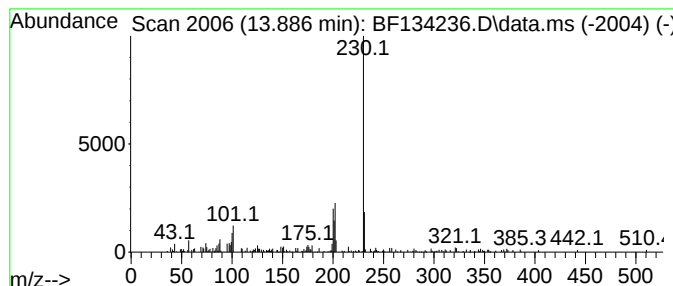
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 7H-Benz[de]anthracen-7-one Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	2.27 ng	48776	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	93
2			7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	89
3			1-Pyrenecarboxaldehyde	230	C17H10O	003029-19-4	83
4			6H-Benz[de]anthracen-6-one	230	C17H10O	080252-14-8	74
5			4-Pyrenecarbaldehyde	230	C17H10O	022245-51-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071123\
Data File : BF134236.D
Acq On : 12 Jul 2023 03:54
Operator : CG\JU
Sample : 03375-07 5X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3(0-2)

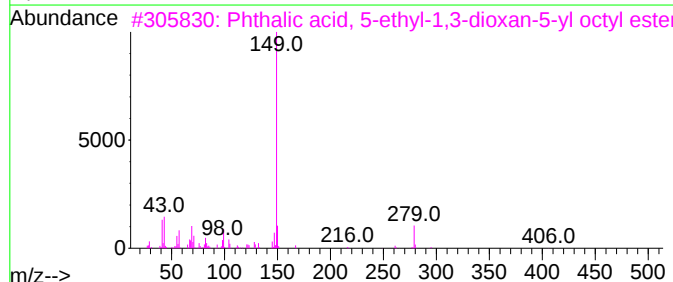
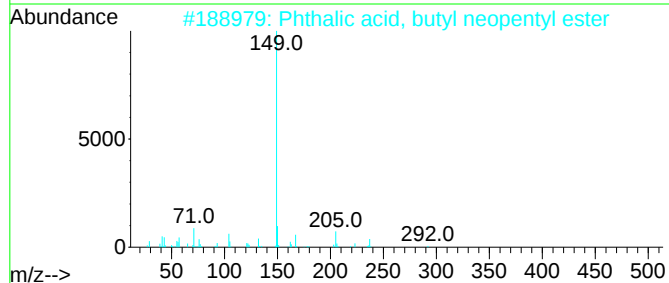
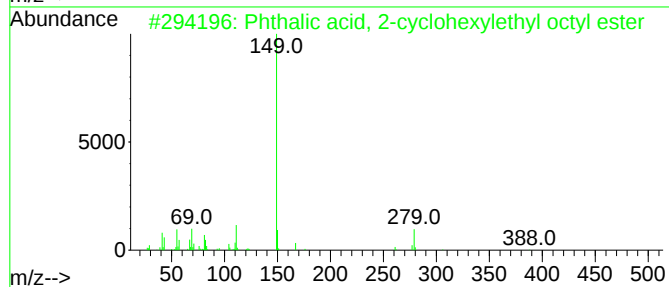
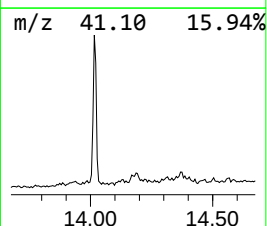
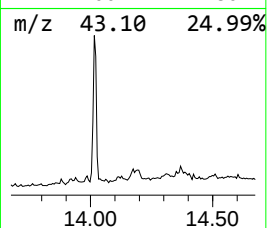
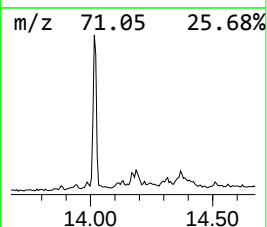
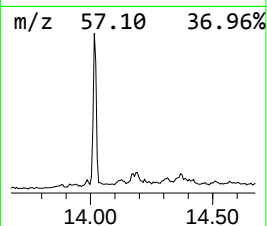
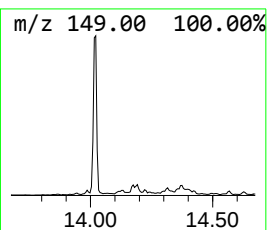
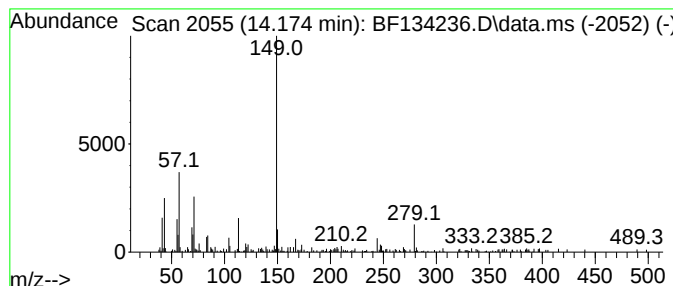
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Phthalic acid, 2-cyclohexyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.174	2.44 ng	52372	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic acid, 2-cyclohexylethyl...	388	C24H36O4	1000309-87-8	72
2			Phthalic acid, butyl neopentyl e...	292	C17H24O4	1000309-03-7	70
3			Phthalic acid, 5-ethyl-1,3-dioxa...	406	C23H34O6	1010415-48-4	64
4			Phthalic acid, butyl 2,7-dimethy...	356	C22H28O4	1010315-49-0	62
5			Phthalic acid, 2,7-dimethyloct-7...	356	C22H28O4	1000315-49-7	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071123\
Data File : BF134236.D
Acq On : 12 Jul 2023 03:54
Operator : CG\JU
Sample : 03375-07 5X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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
n-Hexadecanoic ...	11.910	5.8	ng	151870	4	11.380	522735	20.0
1,2-Benzenedica...	11.945	2.0	ng	52655	4	11.380	522735	20.0
9,10-Anthracene...	12.210	3.0	ng	78789	4	11.380	522735	20.0
unknown12.698	12.698	2.0	ng	52995	4	11.380	522735	20.0
Pyrene, 4-methyl-	13.269	2.7	ng	57043	5	14.039	428841	20.0
11H-Benzo[a]flu...	13.680	3.6	ng	77410	5	14.039	428841	20.0
7H-Benz[de]anth...	13.886	2.3	ng	48776	5	14.039	428841	20.0
Phthalic acid, ...	14.174	2.4	ng	52372	5	14.039	428841	20.0