

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042523\
 Data File : BF133045.D
 Acq On : 26 Apr 2023 00:32
 Operator : CG\JU
 Sample : 02390-07
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SPC-2WC-23-04-17

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-BF042123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133045.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.934	476	484	495	rBV	146182	209164	4.49%	0.482%
2	5.351	551	555	559	rBV	3931372	3989725	85.69%	9.187%
3	6.381	725	730	733	rBV	4143633	4140037	88.92%	9.533%
4	6.581	757	764	768	rBV3	41852	69636	1.50%	0.160%
5	6.739	787	791	794	rBV	1612907	1231525	26.45%	2.836%
6	7.304	880	887	890	rBV	3159872	2794246	60.01%	6.434%
7	8.022	1005	1009	1012	rBV	2015631	1612058	34.62%	3.712%
8	9.098	1188	1192	1195	rBV	5180027	4655947	100.00%	10.721%
9	9.775	1303	1307	1310	rBV	2293817	1757831	37.75%	4.048%
10	10.486	1423	1428	1432	rBV	335638	280107	6.02%	0.645%
11	10.563	1436	1441	1444	rBV	2953633	2621447	56.30%	6.036%
12	11.210	1549	1551	1555	rBV4	44286	52454	1.13%	0.121%
13	11.257	1555	1559	1561	rVV	1883803	1615697	34.70%	3.720%
14	11.280	1561	1563	1565	rVV	202849	153031	3.29%	0.352%
15	11.327	1568	1571	1573	rVB2	66645	54767	1.18%	0.126%
16	11.363	1574	1577	1580	rBV4	32472	52552	1.13%	0.121%
17	11.604	1614	1618	1621	rVB3	84245	95475	2.05%	0.220%
18	11.792	1646	1650	1654	rBV2	611685	638617	13.72%	1.470%
19	11.910	1668	1670	1672	rBV2	64317	53982	1.16%	0.124%
20	12.045	1690	1693	1695	rBV3	107201	106935	2.30%	0.246%
21	12.068	1695	1697	1700	rVB	214968	183788	3.95%	0.423%
22	12.463	1761	1764	1768	rBV	434792	371040	7.97%	0.854%
23	12.580	1779	1784	1787	rBV4	246054	340950	7.32%	0.785%
24	12.692	1800	1803	1805	rVB	322249	240015	5.16%	0.553%
25	12.845	1825	1829	1832	rBV	4127430	3626362	77.89%	8.350%
26	13.892	2003	2007	2010	rBV	1373578	1388936	29.83%	3.198%
27	14.033	2028	2031	2034	rBV	648410	523644	11.25%	1.206%
28	14.110	2040	2044	2047	rBV	3537698	3629434	77.95%	8.357%
29	14.262	2067	2070	2076	rBV	1072982	920436	19.77%	2.119%
30	14.909	2177	2180	2183	rBV	191130	278708	5.99%	0.642%
31	15.004	2193	2196	2201	rVB2	566202	653474	14.04%	1.505%
32	15.086	2207	2210	2214	rVB	421412	425025	9.13%	0.979%
33	15.192	2226	2228	2235	rVB	228596	302571	6.50%	0.697%
34	15.315	2245	2249	2253	rVB	929427	983809	21.13%	2.265%
35	16.721	2482	2488	2500	rVB	682625	1343730	28.86%	3.094%
36	17.698	2647	2654	2667	rVB	856987	2031524	43.63%	4.678%

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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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

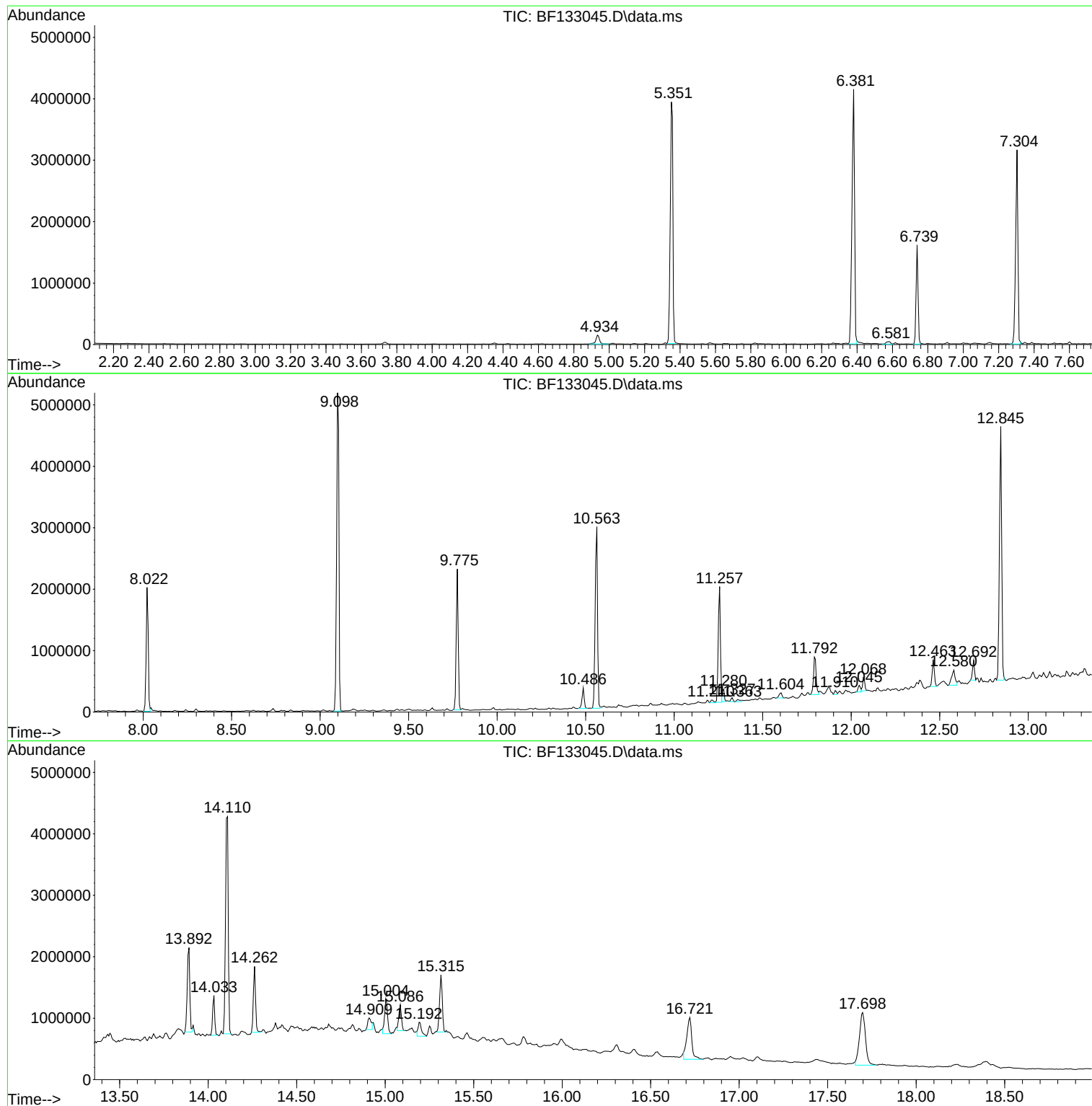
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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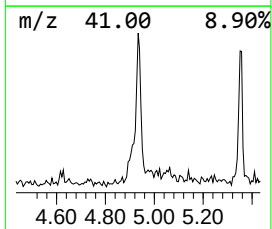
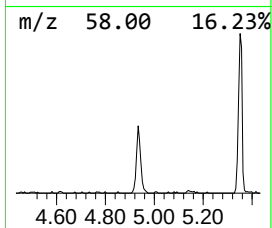
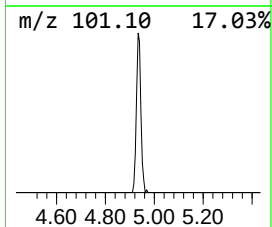
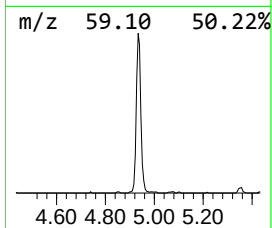
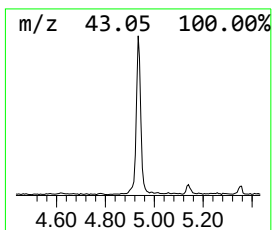
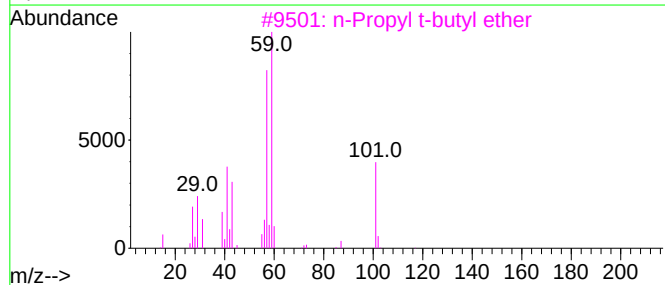
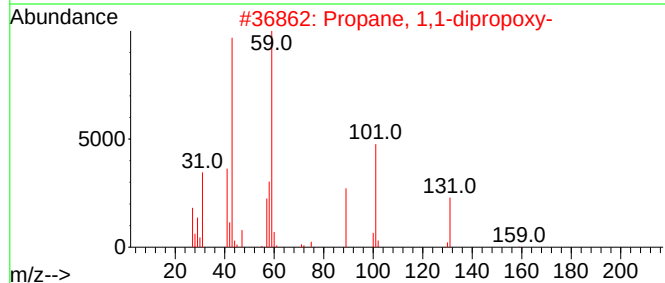
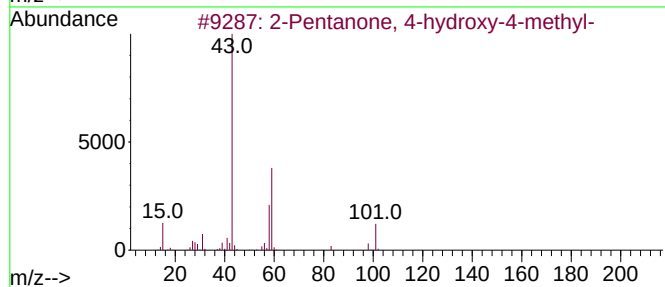
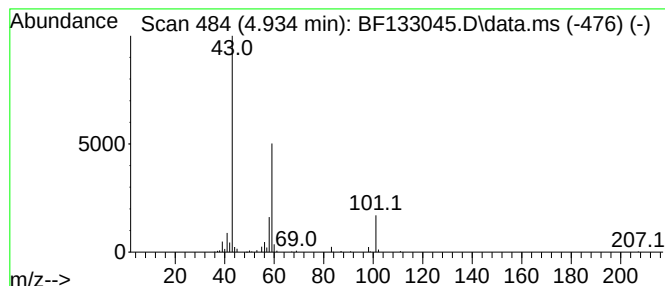
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.934	3.40 ng	209164	1,4-Dichlorobenzene-d4	6.739

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	38	
3	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33	
4	4-Methoxy-1-pentene	100	C6H12O	098386-09-5	23	
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12	



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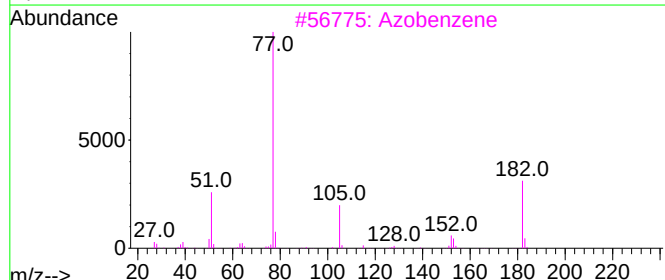
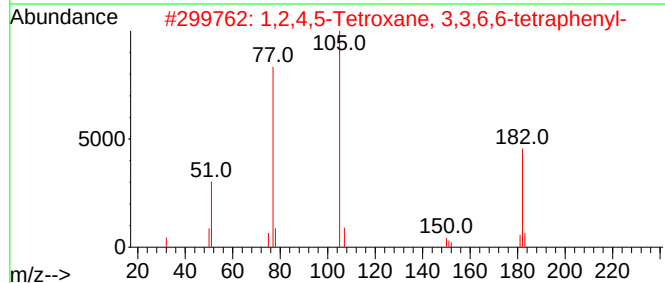
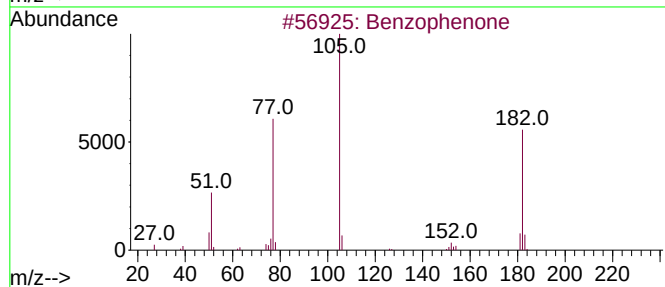
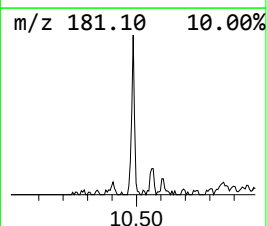
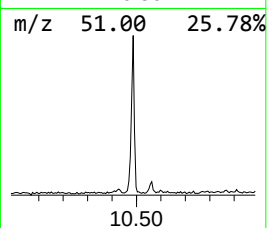
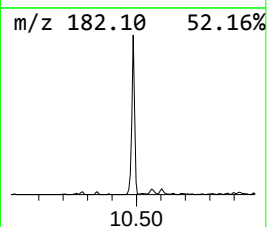
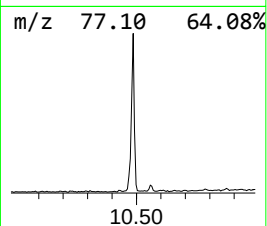
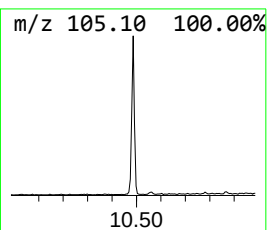
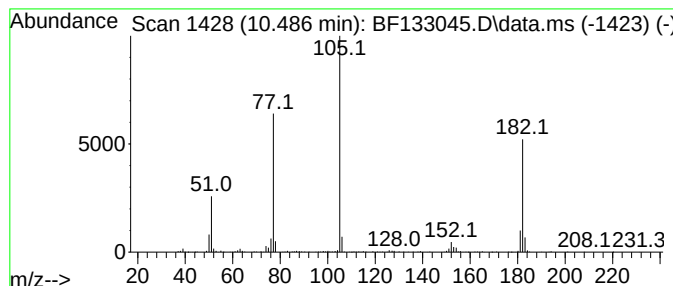
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.486	3.19 ng	280107	Acenaphthene-d10	9.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
3			Azobenzene	182	C12H10N2	000103-33-3	64
4			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
5			2-(2-Oxo-2-phenyl-ethyl)-malon...	184	C11H8N2O	1000296-76-9	47



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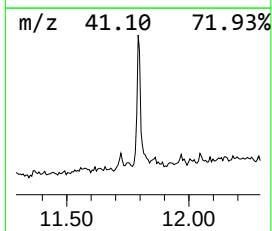
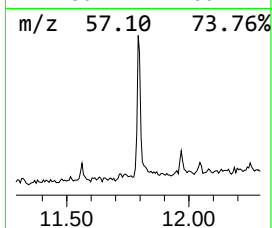
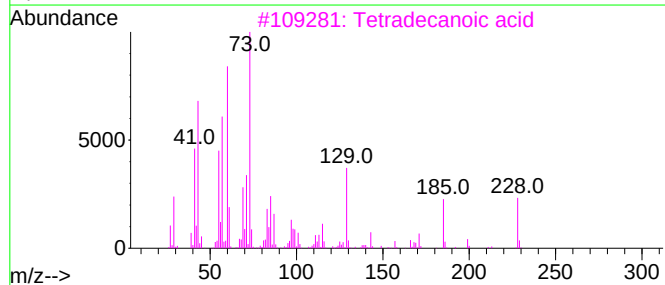
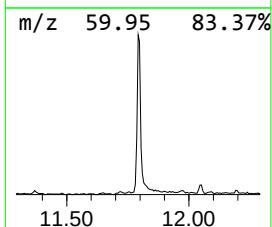
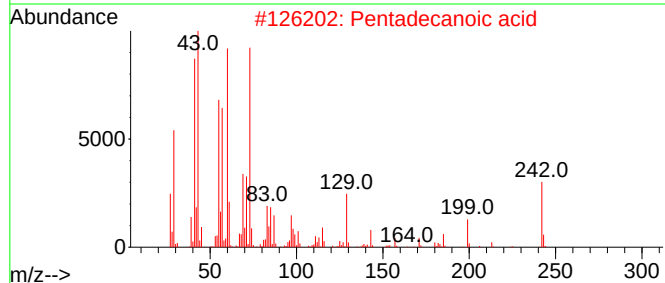
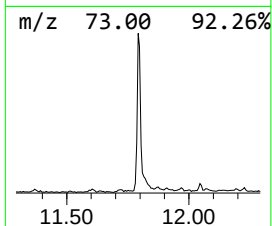
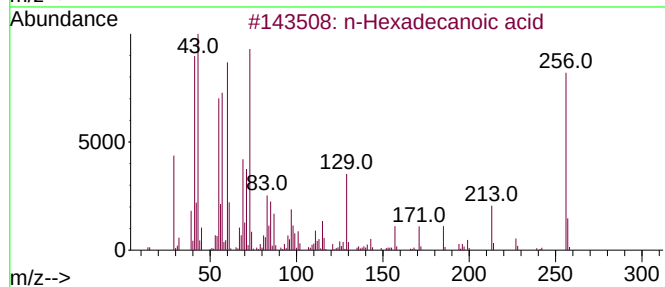
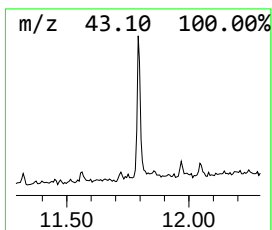
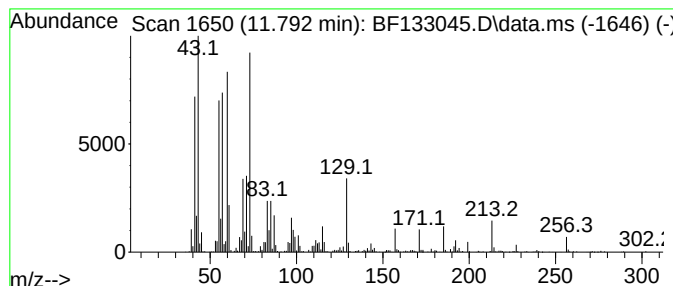
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.792	7.91 ng	638617	Phenanthrene-d10	11.257

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	80
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			Tridecanoic acid	214	C13H26O2	000638-53-9	74
5			Dodecanoic acid	200	C12H24O2	000143-07-7	59



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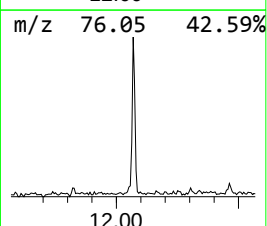
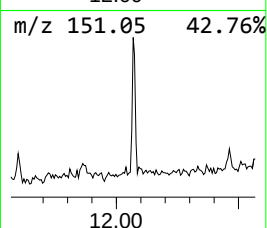
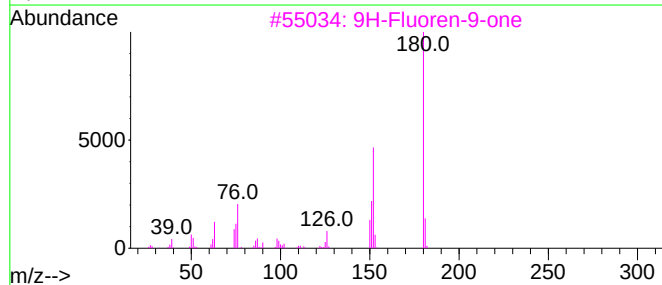
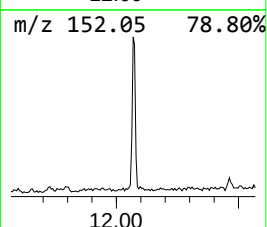
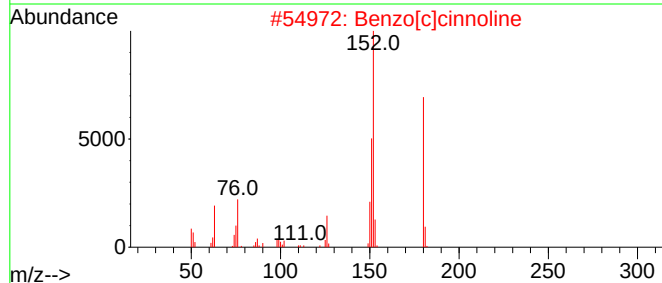
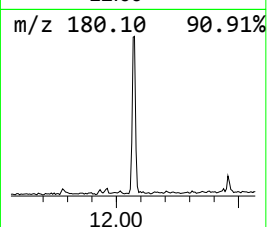
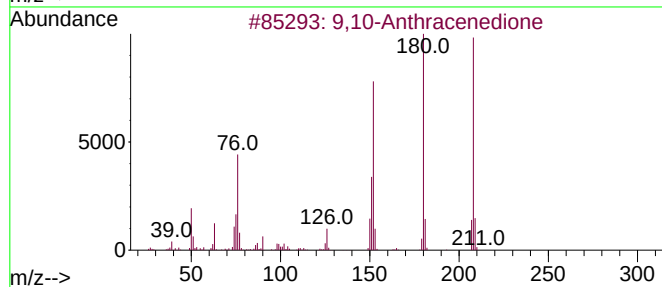
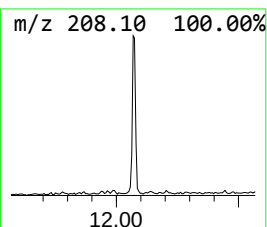
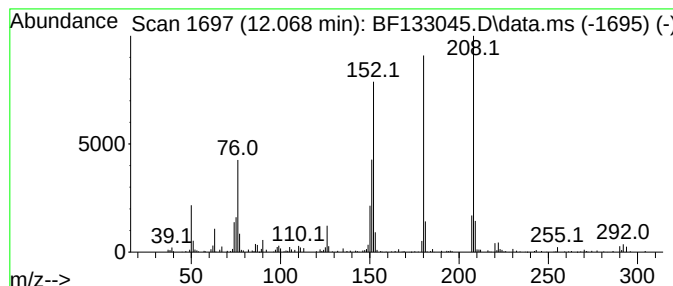
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 4 9,10-Anthracenedione Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.069	2.28 ng	183788	Phenanthrene-d10	11.257

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	60
3		9H-Fluoren-9-one	180	C13H8O	000486-25-9	58
4		1H-Phenalen-1-one	180	C13H8O	000548-39-0	55
5		1,4-Anthracenedione	208	C14H8O2	000635-12-1	46



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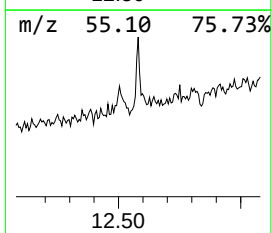
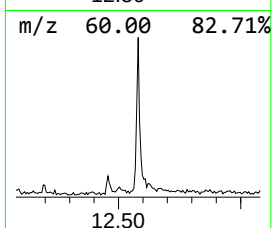
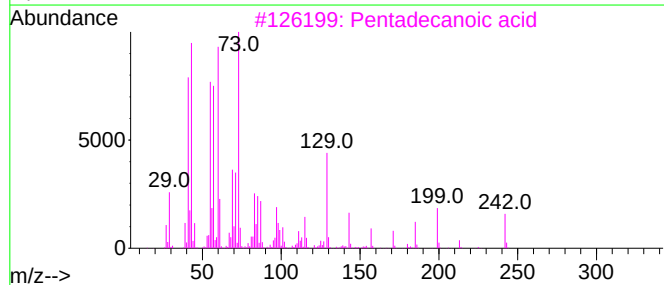
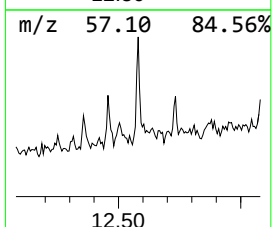
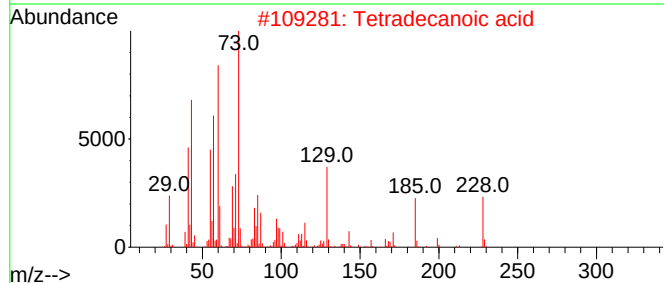
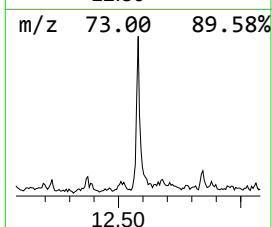
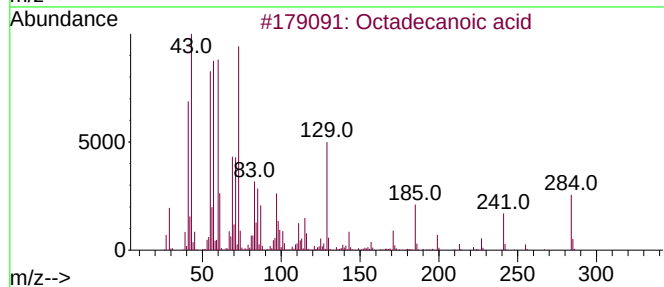
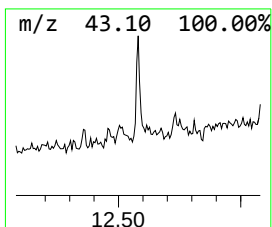
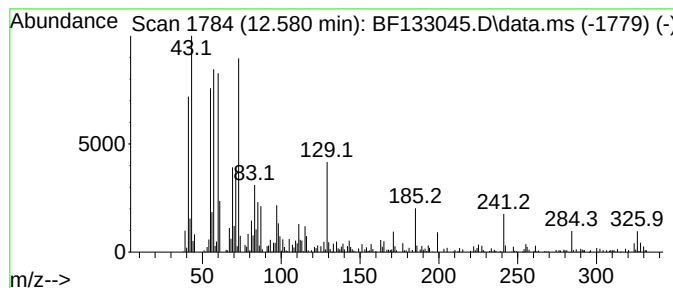
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.580	4.91 ng	340950	Chrysene-d12	13.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Undecanoic acid	186	C11H22O2	000112-37-8	68
5			Heneicosanoic acid	326	C21H42O2	002363-71-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042523\
Data File : BF133045.D
Acq On : 26 Apr 2023 00:32
Operator : CG\JU
Sample : 02390-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SPC-2WC-23-04-17

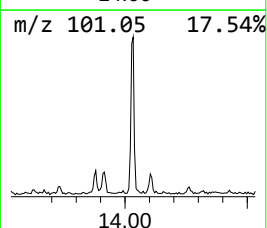
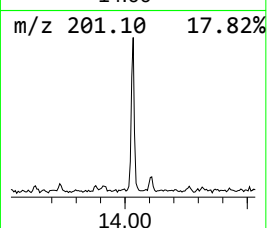
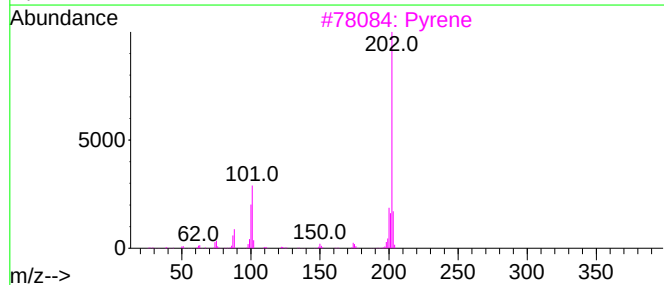
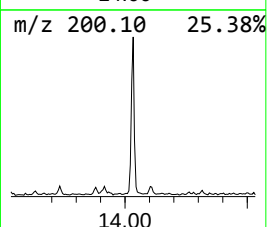
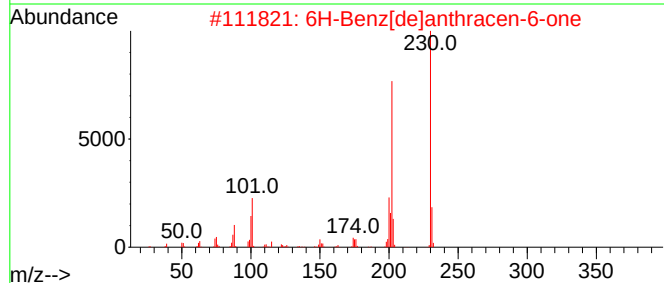
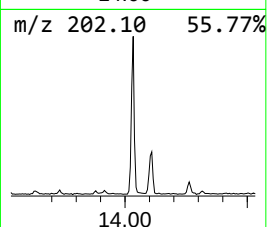
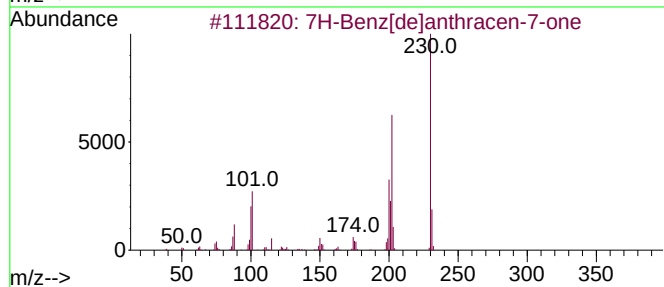
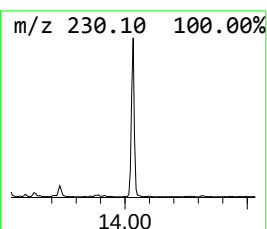
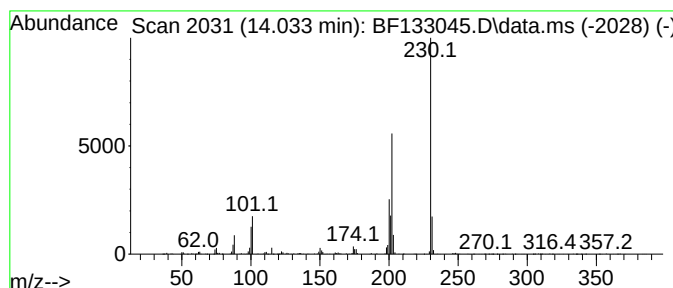
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.033	7.54 ng	523644	Chrysene-d12	13.892

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	98
2		6H-Benz[de]anthracen-6-one	230	C17H10O	080252-14-8	96
3		Pyrene	202	C16H10	000129-00-0	83
4		11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	83
5		1-Pyrenecarboxaldehyde	230	C17H10O	003029-19-4	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042523\
Data File : BF133045.D
Acq On : 26 Apr 2023 00:32
Operator : CG\JU
Sample : 02390-07
Misc :
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ClientSampleId :
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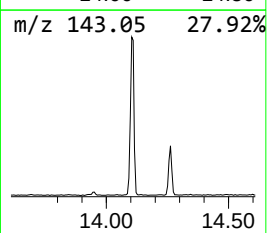
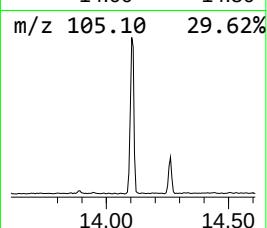
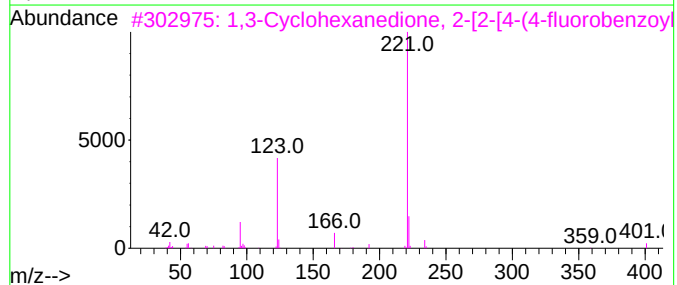
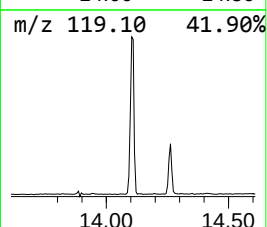
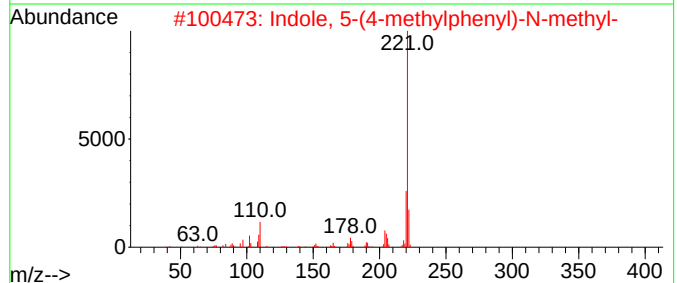
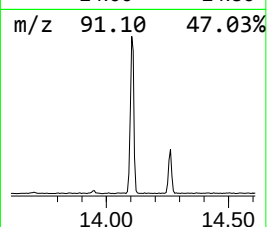
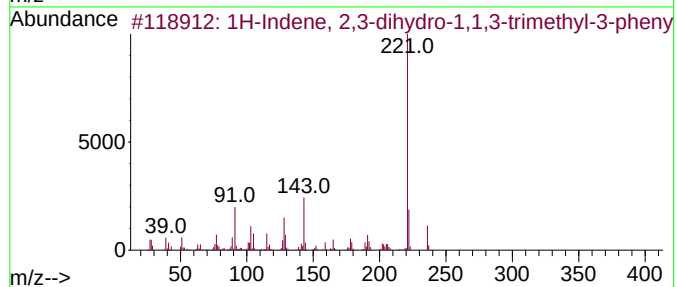
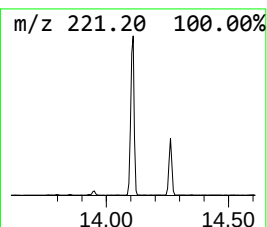
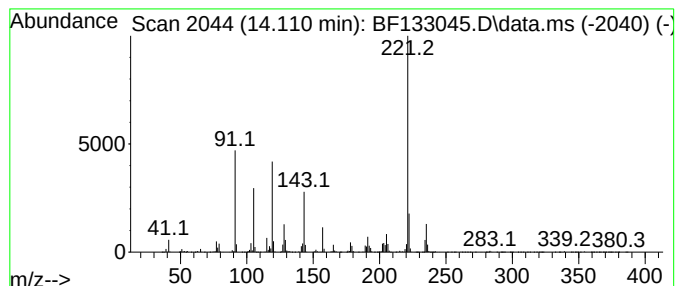
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown14.110 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.110	52.26 ng	3629430	Chrysene-d12	13.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	46
2			Indole, 5-(4-methylphenyl)-N-met...	221	C16H15N	1000380-54-7	43
3			1,3-Cyclohexanedione, 2-[2-[4-(4...	401	C22H28FN3O3	339310-26-8	38
4			Benz[j]isoquinoline, 3,6,8-trime...	221	C16H15N	061171-16-2	38
5			2-Mercapto-4,6-dimethylnicotinon...	236	C11H16N2SSi	1000332-43-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042523\
Data File : BF133045.D
Acq On : 26 Apr 2023 00:32
Operator : CG\JU
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ClientSampleId :
SPC-2WC-23-04-17

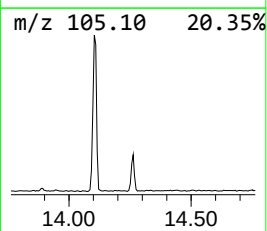
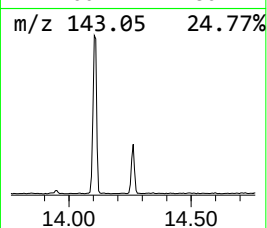
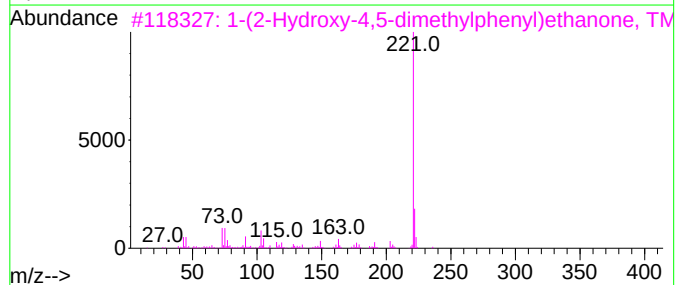
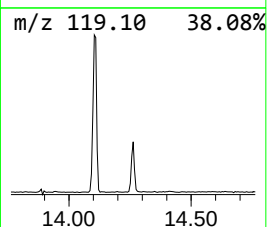
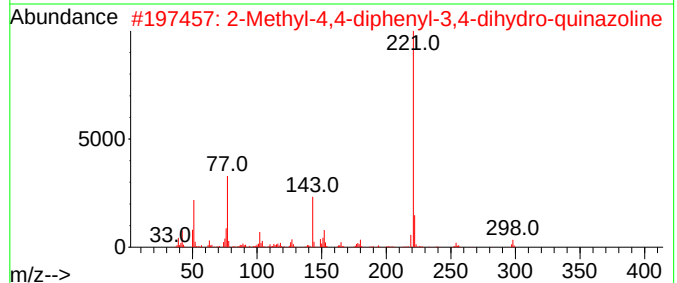
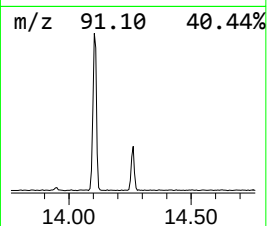
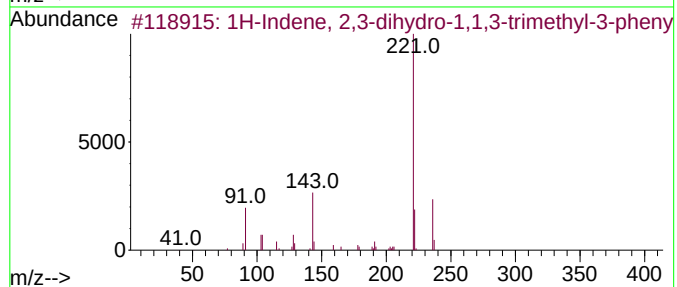
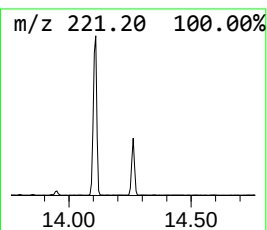
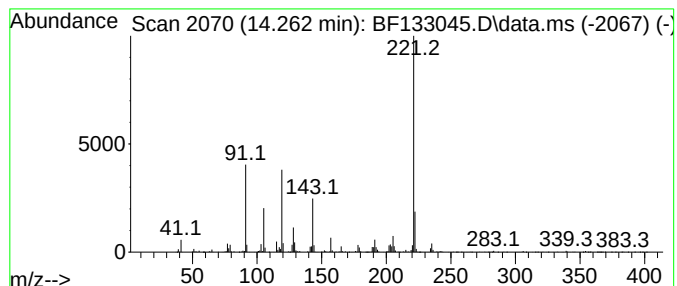
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown14.262 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.262	13.25 ng	920436	Chrysene-d12	13.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	47
2			2-Methyl-4,4-diphenyl-3,4-dihydr...	298	C21H18N2	1000300-40-0	43
3			1-(2-Hydroxy-4,5-dimethylphenyl)...	236	C13H20O2Si	1000484-73-7	38
4			Oxazole, 2,5-diphenyl-	221	C15H11NO	000092-71-7	38
5			1-(2-Hydroxy-5-methylphenyl)prop...	236	C13H20O2Si	1000506-71-9	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042523\
Data File : BF133045.D
Acq On : 26 Apr 2023 00:32
Operator : CG\JU
Sample : 02390-07
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ClientSampleId :
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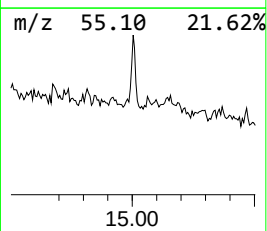
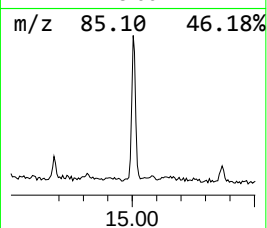
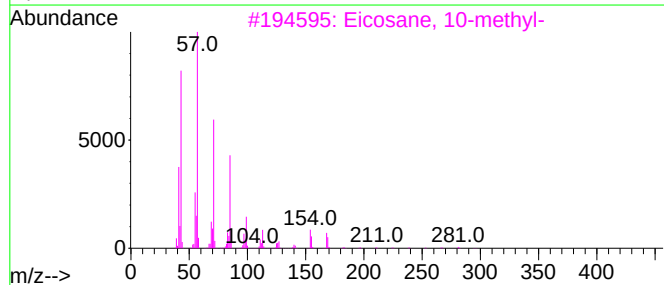
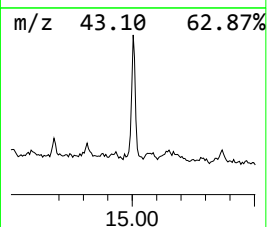
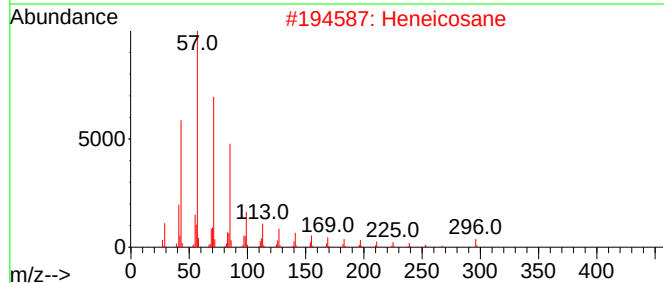
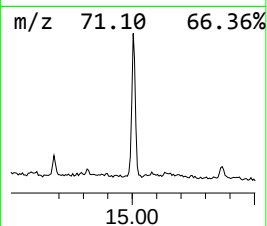
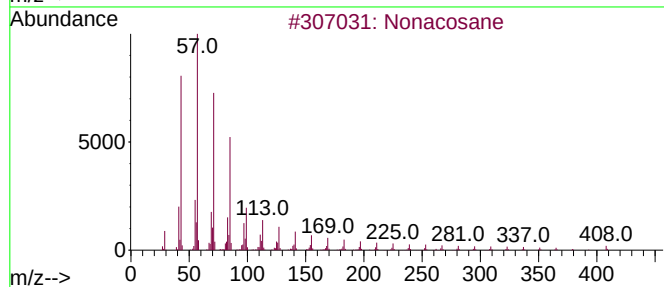
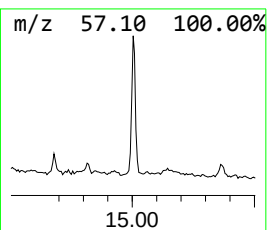
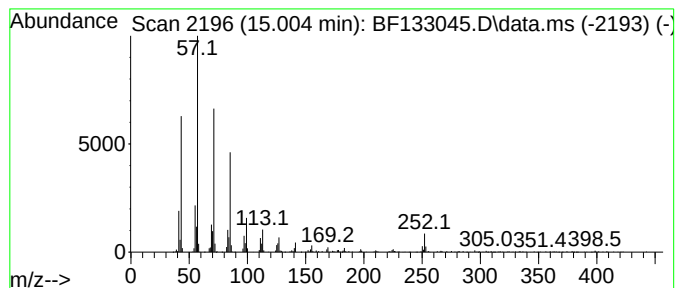
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Nonacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.004	13.28 ng	653474	Perylene-d12	15.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonacosane	408	C29H60	000630-03-5	93
2			Heneicosane	296	C21H44	000629-94-7	91
3			Eicosane, 10-methyl-	296	C21H44	054833-23-7	91
4			Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	91
5			Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042523\
Data File : BF133045.D
Acq On : 26 Apr 2023 00:32
Operator : CG\JU
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ClientSampleId :
SPC-2WC-23-04-17

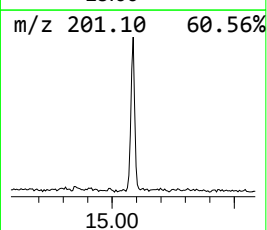
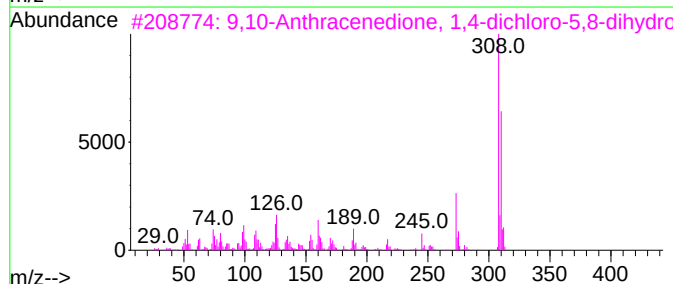
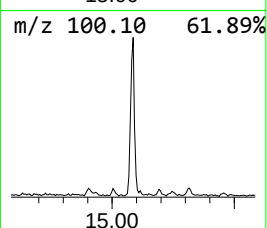
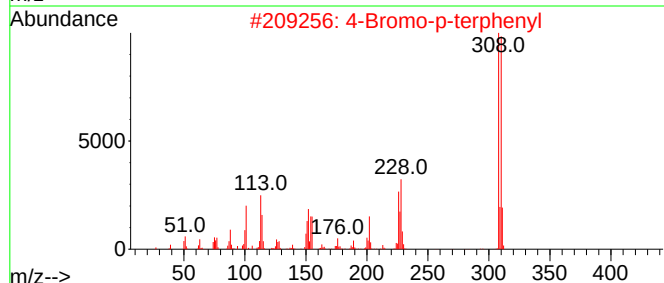
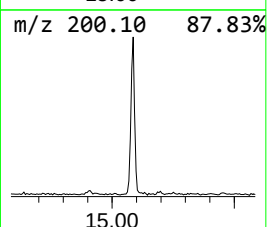
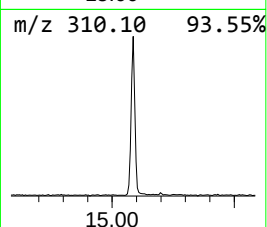
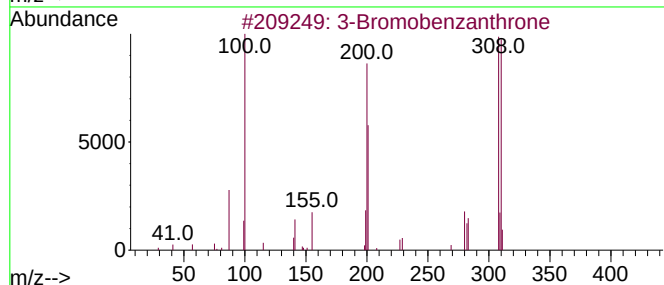
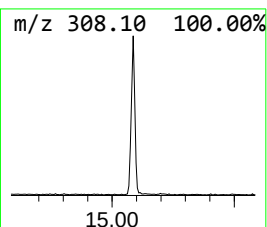
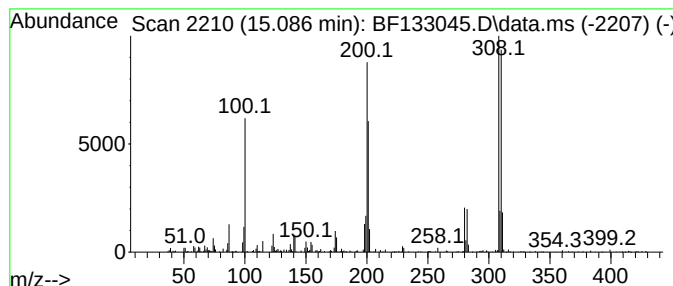
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 3-Bromobenzanthrone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.086	8.64 ng	425025	Perylene-d12	15.315

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Bromobenzanthrone	308	C17H9BrO	000081-96-9	94
2		4-Bromo-p-terphenyl	308	C18H13Br	001762-84-1	45
3		9,10-Anthracenedione, 1,4-dichlo...	308	C14H6Cl2O4	002832-30-6	35
4		9,10-Anthracenedione, 1,5-dichlo...	308	C14H6Cl2O4	006837-97-4	25
5		bis(4-Methoxyphenyl)(5-methyl-2-...	308	C20H20O3	1000440-63-6	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042523\
Data File : BF133045.D
Acq On : 26 Apr 2023 00:32
Operator : CG\JU
Sample : 02390-07
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ALS Vial : 14 Sample Multiplier: 1

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ClientSampleId :
SPC-2WC-23-04-17

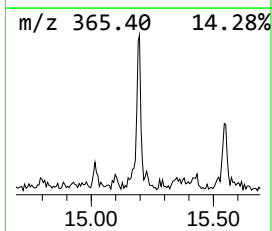
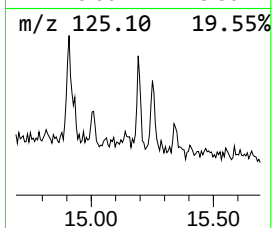
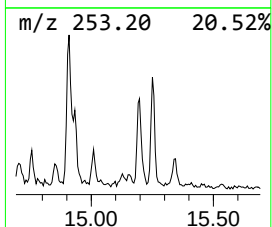
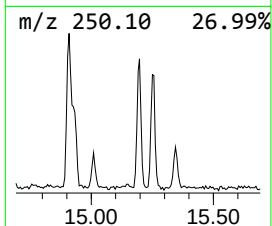
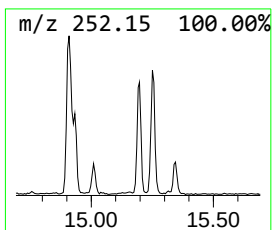
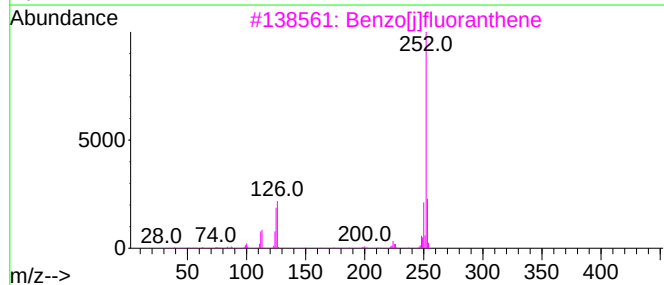
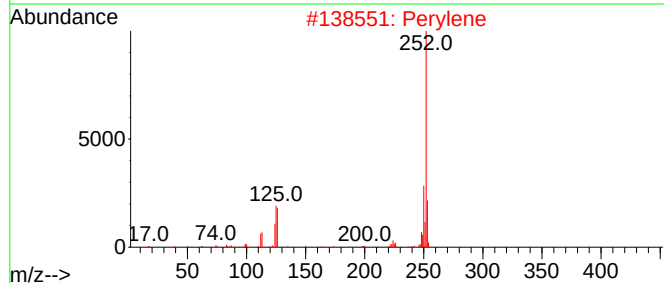
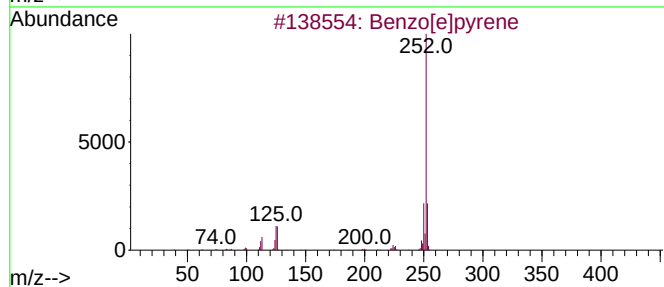
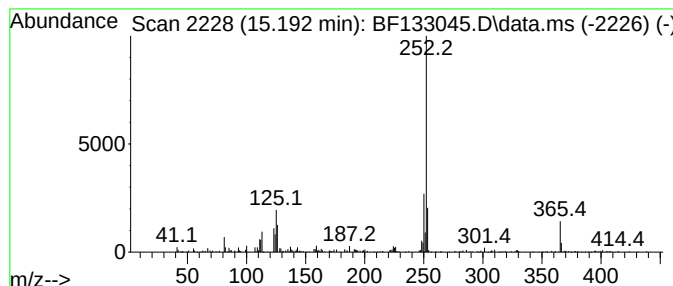
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.192	6.15 ng	302571	Perylene-d12	15.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	93
2			Perylene	252	C20H12	000198-55-0	93
3			Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	92
5			Benzo[a]pyrene	252	C20H12	000050-32-8	92



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042523\
Data File : BF133045.D
Acq On : 26 Apr 2023 00:32
Operator : CG\JU
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ALS Vial : 14 Sample Multiplier: 1

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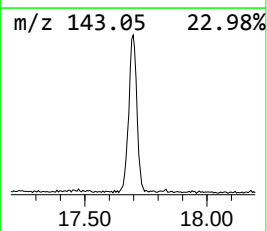
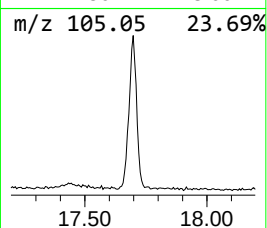
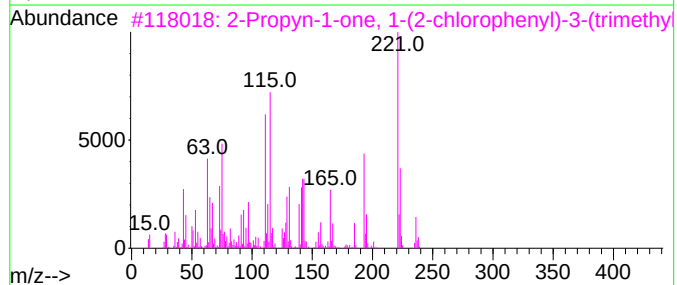
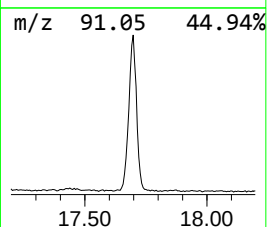
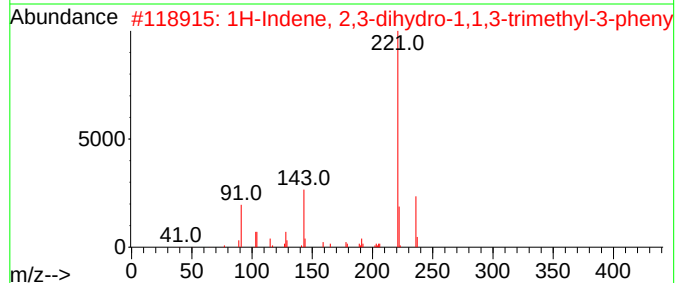
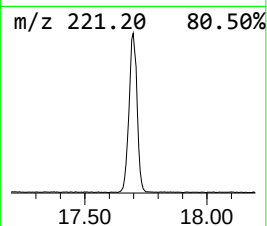
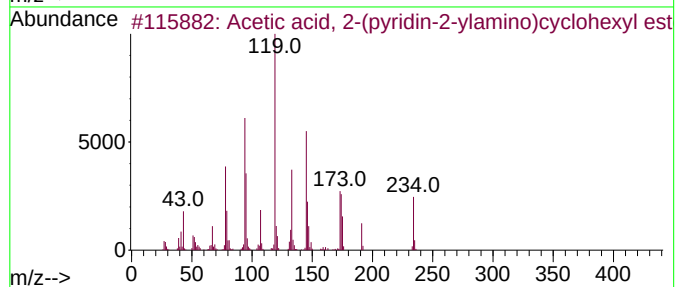
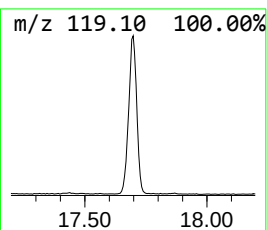
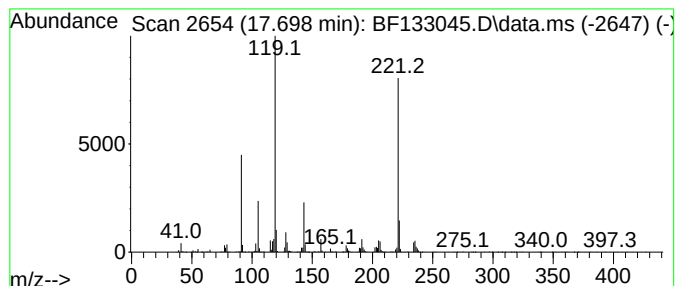
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 unknown17.698 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.698	41.30 ng	2031520	Perylene-d12	15.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, 2-(pyridin-2-ylamin...	234	C13H18N2O2	1000185-40-1	42
2			1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	38
3			2-Propyn-1-one, 1-(2-chloropheny...	236	C12H13ClOSi	1000460-97-3	35
4			Dicumyl peroxide	270	C18H22O2	000080-43-3	35
5			2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042523\
Data File : BF133045.D
Acq On : 26 Apr 2023 00:32
Operator : CG\JU
Sample : 02390-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPC-2WC-23-04-17

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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
2-Pentanone, 4-...	4.934	3.4	ng	209164	1	6.739	1231530	20.0
Benzophenone	10.486	3.2	ng	280107	3	9.775	1757830	20.0
n-Hexadecanoic ...	11.792	7.9	ng	638617	4	11.257	1615700	20.0
9,10-Anthracene...	12.069	2.3	ng	183788	4	11.257	1615700	20.0
Octadecanoic acid	12.580	4.9	ng	340950	5	13.892	1388940	20.0
7H-Benz[de]anth...	14.033	7.5	ng	523644	5	13.892	1388940	20.0
unknown14.110	14.110	52.3	ng	3629430	5	13.892	1388940	20.0
unknown14.262	14.262	13.3	ng	920436	5	13.892	1388940	20.0
Nonacosane	15.004	13.3	ng	653474	6	15.315	983809	20.0
3-Bromobenzanth...	15.086	8.6	ng	425025	6	15.315	983809	20.0
Benzo[e]pyrene	15.192	6.2	ng	302571	6	15.315	983809	20.0
unknown17.698	17.698	41.3	ng	2031520	6	15.315	983809	20.0