LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042123\
Data File : BF132984.D
Acq On : 21 Apr 2023 23:09
Operator : CG\JU
Sample : 02390-03 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPC-1WC-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: BF132984.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.757	275	284	289	rBV	39869	62612	2.50%	0.210%
2	4.369	383	388	397	rBV	43026	55523	2.22%	0.186%
3	4.940	474	485	495	rBV	493283	561833	22.47%	1.884%
4	5.363	552	557	560	rVB	2600615	2431230	97.25%	8.155%
5	5.581	589	594	598	rBV3	30222	47953	1.92%	0.161%
6	5.828	633	636	643	rBV	75853	97506	3.90%	0.327%
7	5.998	660	665	668	rBV	64718	73290	2.93%	0.246%
8	6.387	727	731	734	rBV	2905845	2409932	96.40%	8.083%
9	6.416	734	736	742	rVB4	47501	65300	2.61%	0.219%
10	6.581	760	764	769	rBV4	46453	80312	3.21%	0.269%
11	6.751	789	793	796	rBV	1785505	1336072	53.44%	4.481%
12	7.310	882	888	891	rBV	1846672	1491635	59.66%	5.003%
13	8.034	1007	1011	1014	rBV	2184887	1712748	68.51%	5.745%
14	8.192	1035	1038	1046	rBV	43439	46787	1.87%	0.157%
15	9.110	1190	1194	1197	rVB	3213048	2422798	96.91%	8.126%
16	9.233	1213	1215	1218	rVB	50392	41347	1.65%	0.139%
17	9.345	1231	1234	1236	rBV	34523	44826	1.79%	0.150%
18	9.645	1282	1285	1290	rBV	79583	64700	2.59%	0.217%
19	9.786	1304	1309	1313	rBV	1961966	1641123	65.64%	5.505%
20	9.898	1325	1328	1331	rBV2	33516	46882	1.88%	0.157%
21	10.498	1426	1430	1434	rVB	107022	113710	4.55%	0.381%
22	10.575	1439	1443	1446	rBV	1223176	1107634	44.30%	3.715%
23	10.710	1462	1466	1472	rBV3	61800	104656	4.19%	0.351%
24	10.880	1492	1495	1498	rBV	265644	219155	8.77%	0.735%
25	10.945	1503	1506	1509	rVB3	57864	68331	2.73%	0.229%
26	11.204	1548	1550	1552	rVB	71750	51796	2.07%	0.174%
27	11.269	1558	1561	1564	rBV	1604662	1373500	54.94%	4.607%
28	11.292	1564	1565	1567	rVV	314086	163768	6.55%	0.549%
29	11.345	1571	1574	1576	rVV	83170	79513	3.18%	0.267%
30	11.810	1649	1653	1661	rBV3	361250	472240	18.89%	1.584%
31	12.086	1697	1700	1703	rVB	295981	215526	8.62%	0.723%
32	12.480	1764	1767	1770	rVB	780361	612678	24.51%	2.055%
33	12.710	1803	1806	1808	rVB	551289	423459	16.94%	1.420%
34	12.857	1828	1831	1836	rVB	1912734	1758533	70.34%	5.898%
35	13.904	2005	2009	2012	rBV3	1516049	1734317	69.37%	5.817%
36	13.933	2012	2014	2016	rVB	313729	230061	9.20%	0.772%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042123\
Data File : BF132984.D
Acq On : 21 Apr 2023 23:09
Operator : CG\JU
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Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPC-1WC-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

37	14.010	2024	2027	2031	rVB	670592	608195	24.33%	2.040%
38	14.051	2031	2034	2037	rVB	1094683	880433	35.22%	2.953%
39	14.121	2043	2046	2051	rVB	2783690	2500051	100.00%	8.385%
40	14.280	2070	2073	2076	rBV	649774	619390	24.78%	2.078%
41	15.339	2250	2253	2256	rVB	649442	704677	28.19%	2.364%
42	17.739	2655	2661	2669	rVB	452406	1037990	41.52%	3.482%

Sum of corrected areas: 29814022

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Instrument :
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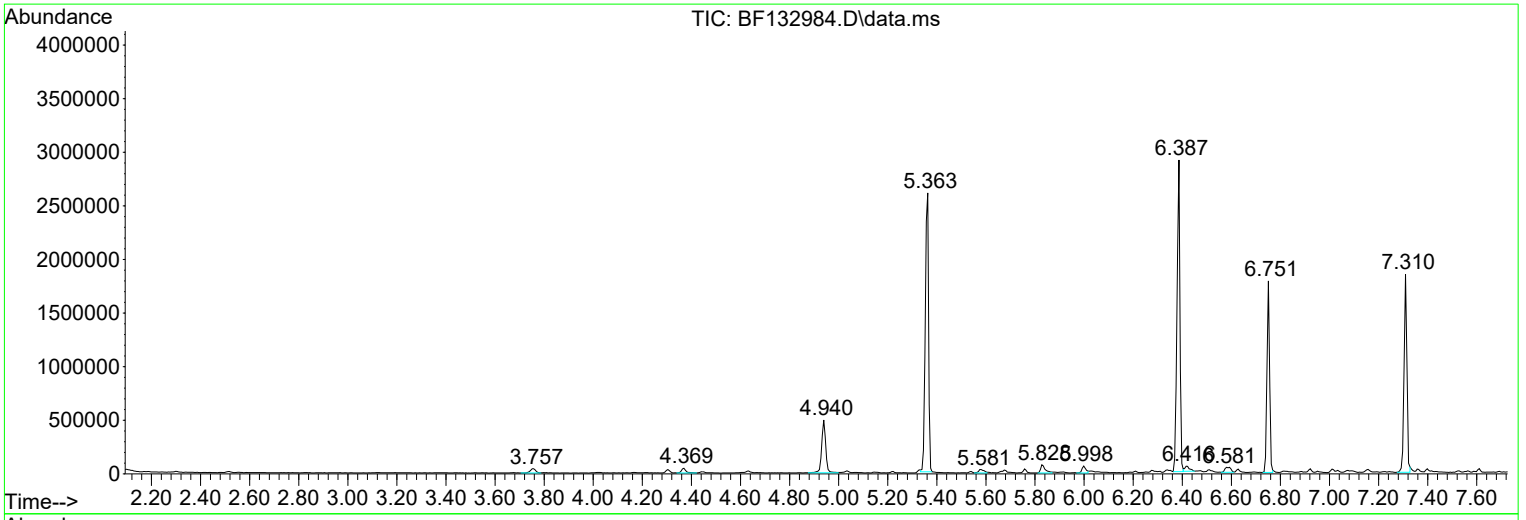
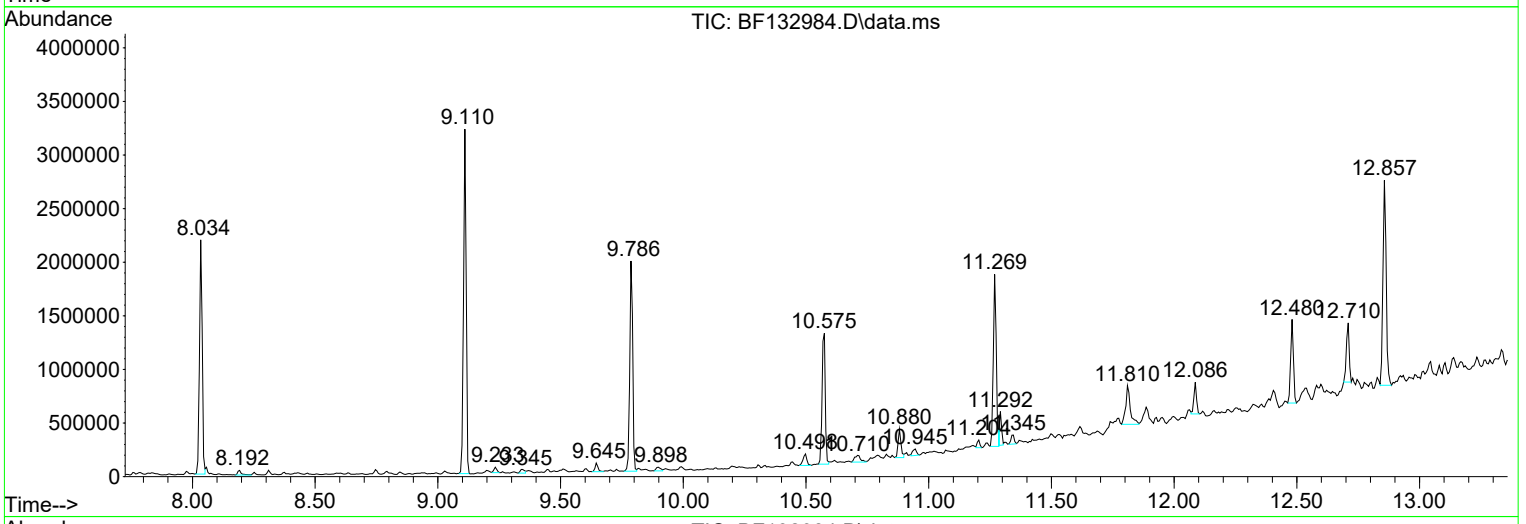
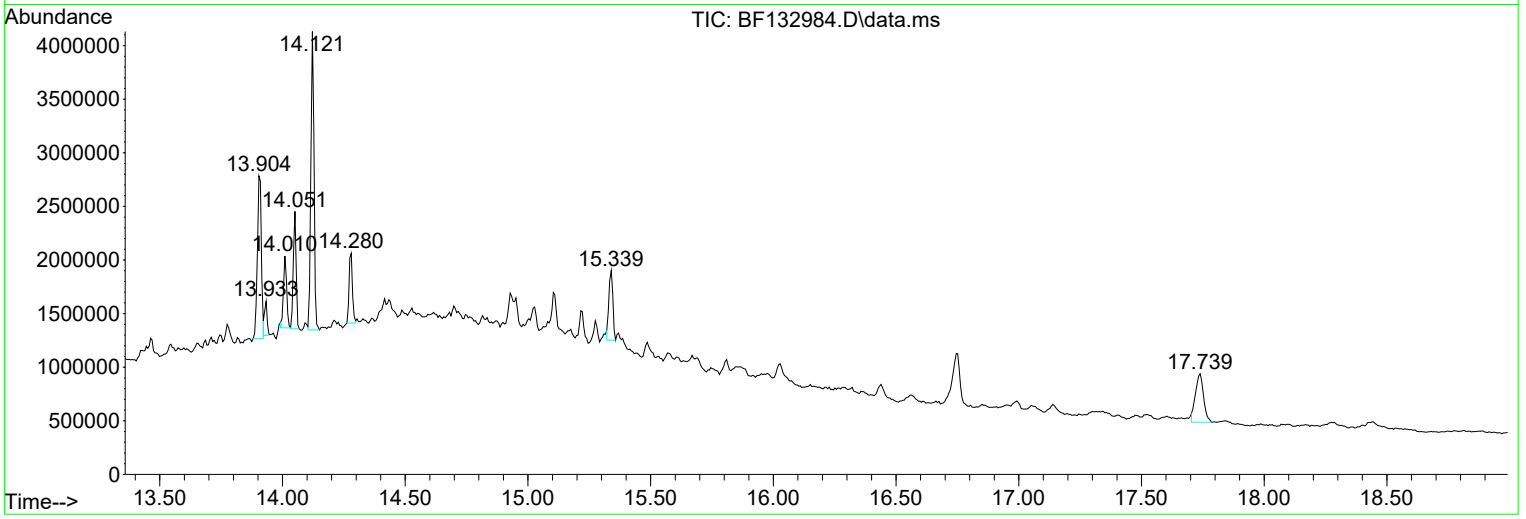
ClientSampleId :
SPC-1WC-23-04-17

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

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







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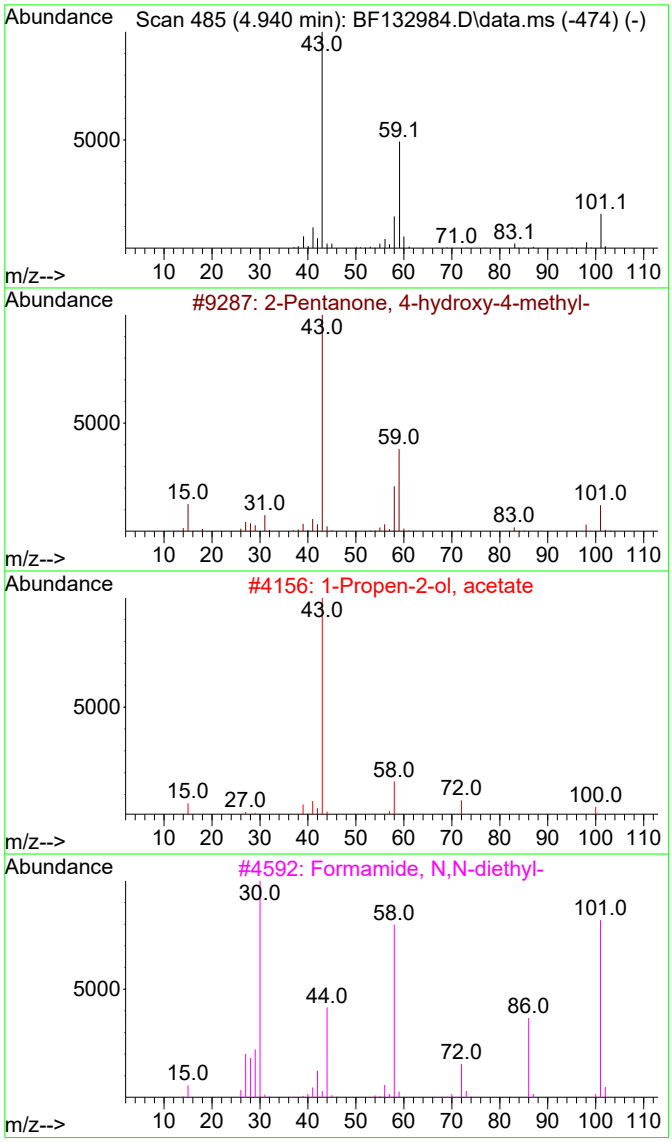
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

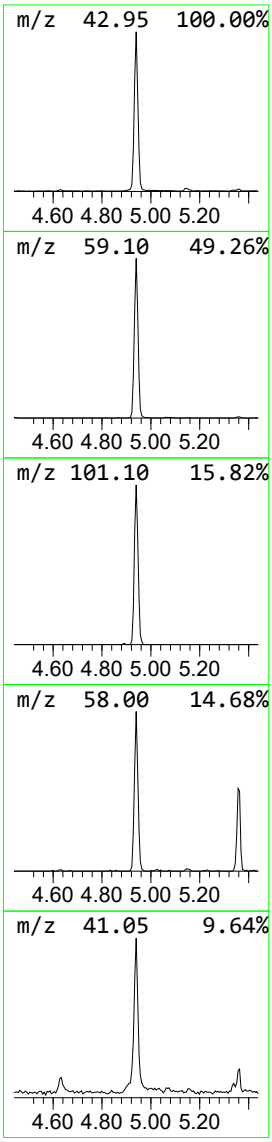
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.940	8.41 ng	561833	1,4-Dichlorobenzene-d4	6.751

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
3	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Butanoic acid, 4-amino-3-hydroxy...	119	C4H9NO3	000924-49-2	9





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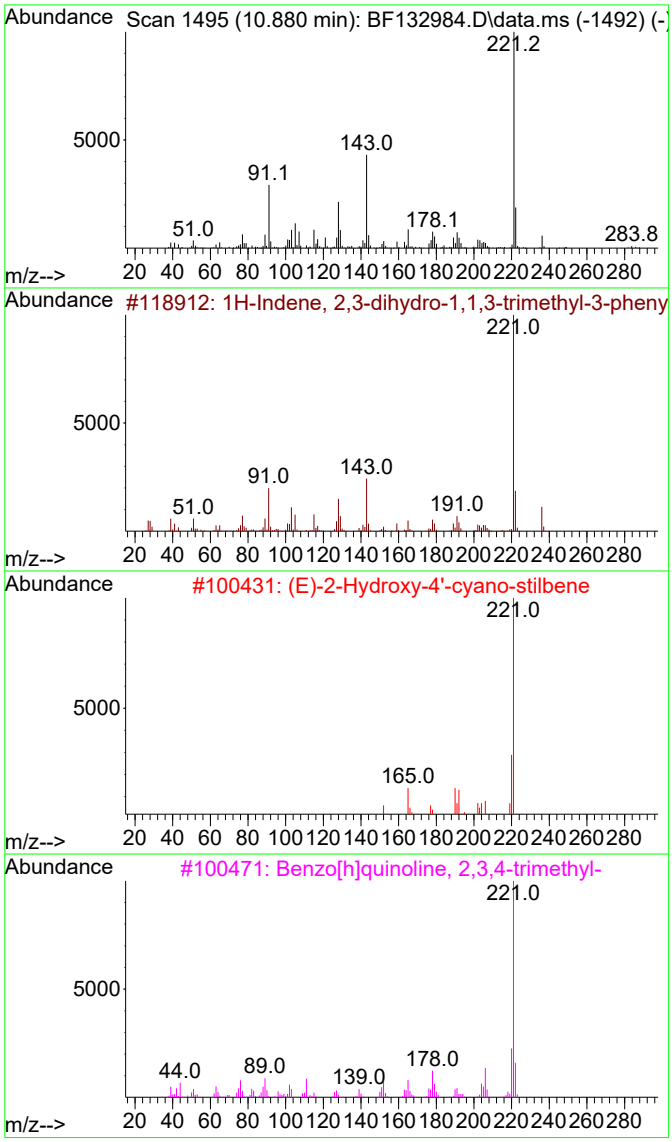
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

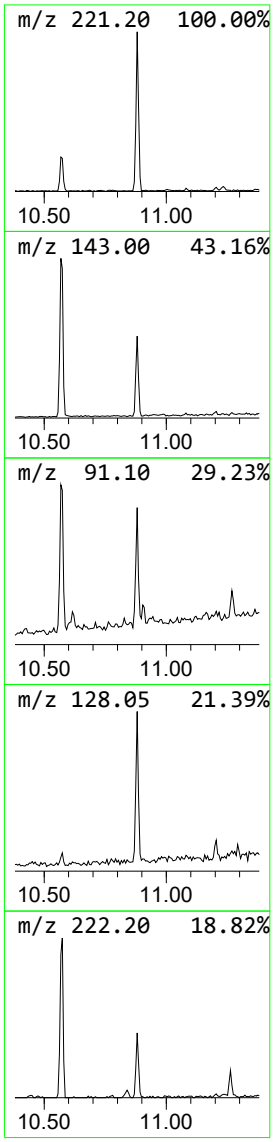
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1H-Indene, 2,3-dihydro-1,1,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.880	3.19 ng	219155	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	93
2	(E)-2-Hydroxy-4'-cyano-stilbene	221	C15H11NO	1000147-85-5	50
3	Benzo[h]quinoline, 2,3,4-trimethyl-	221	C16H15N	063042-66-0	43
4	Ambrox	236	C16H28O	100679-85-4	43
5	Naphthalene, 1,2,3,4-tetrahydro-...	236	C18H20	006196-98-1	38





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Data File : BF132984.D
Acq On : 21 Apr 2023 23:09
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Sample : 02390-03 2X
Misc :
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Instrument :
BNA_F
ClientSampleId :
SPC-1WC-23-04-17

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

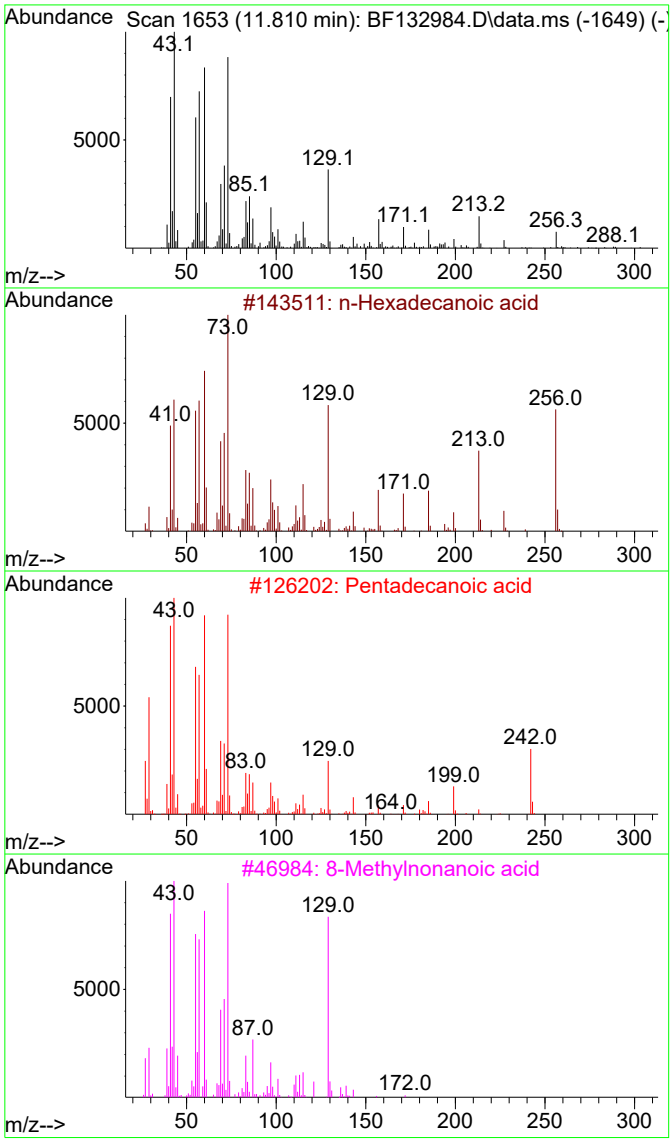
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

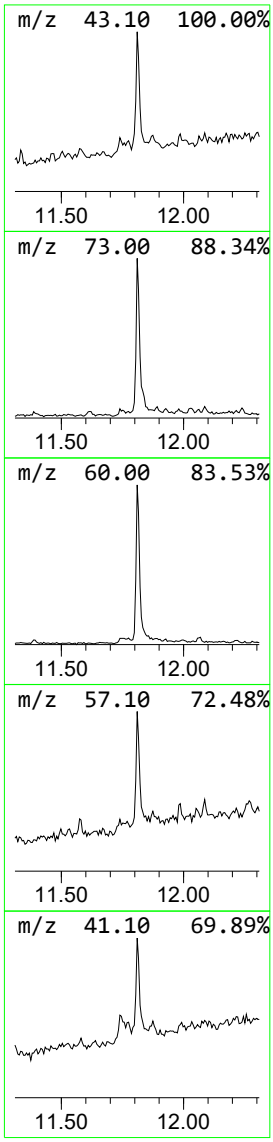
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.810	6.88 ng	472240	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	86
3	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	78
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	Undecanoic acid	186	C11H22O2	000112-37-8	74





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

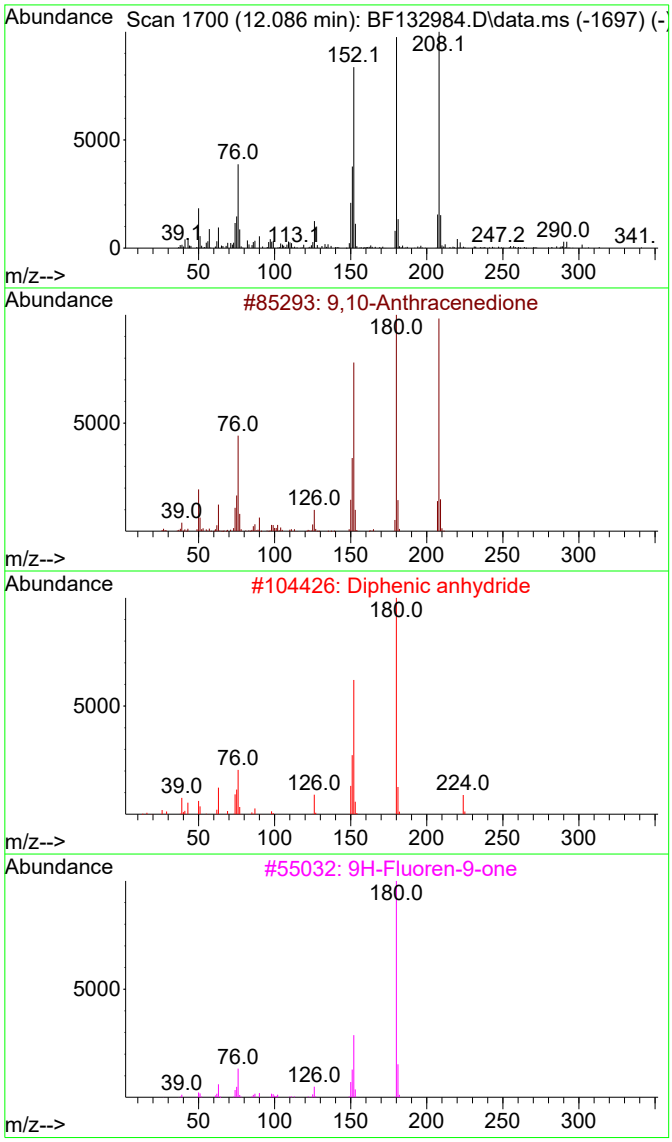
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

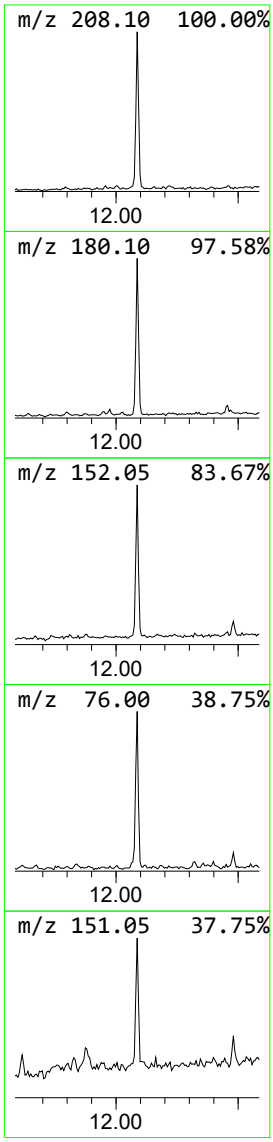
****

Peak Number 4 9,10-Anthracenedione Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.086	3.14 ng	215526	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione	208	C14H8O2	000084-65-1	99
2	Diphenic anhydride	224	C14H8O3	006050-13-1	78
3	9H-Fluoren-9-one	180	C13H8O	000486-25-9	78
4	Anthraquinone-1-carboxylic acid	252	C15H8O4	000602-69-7	72
5	1H-Phenalen-1-one	180	C13H8O	000548-39-0	70





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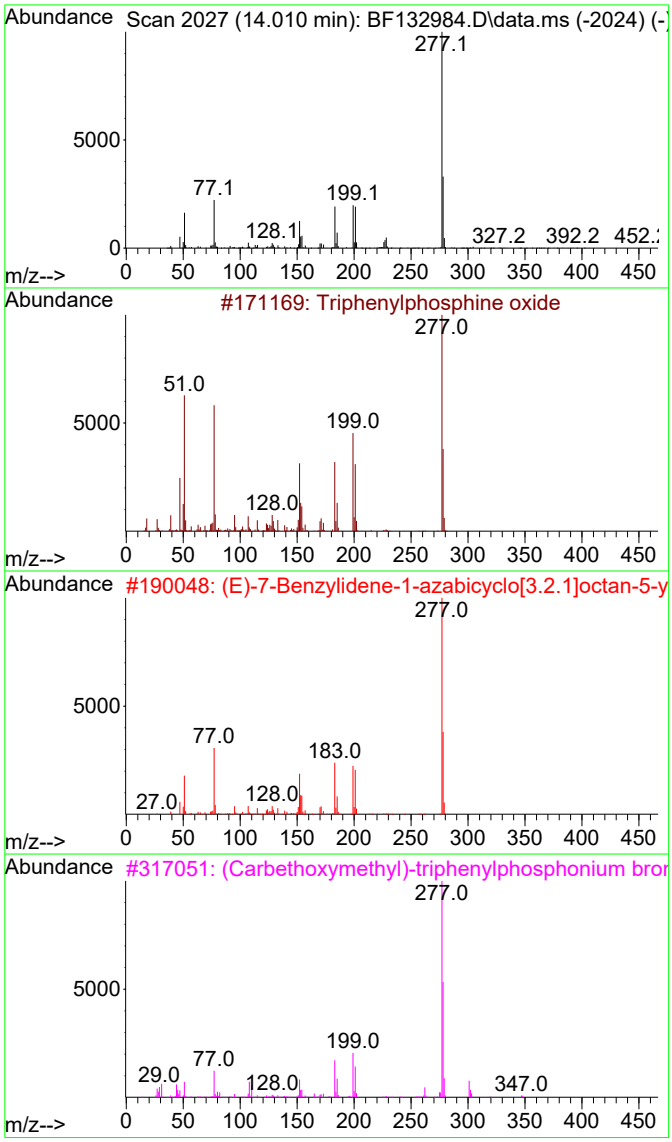
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

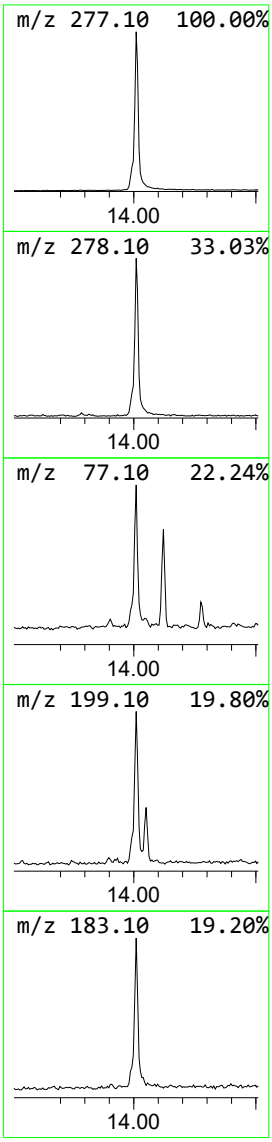
****

Peak Number 5 Triphenylphosphine oxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.010	7.01 ng	608195	Chrysene-d12	13.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	87
3	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	47
4	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	43
5	Silane, dimethyl(dimethylisohexy...	292	C13H32O3Si2	1000346-94-9	17





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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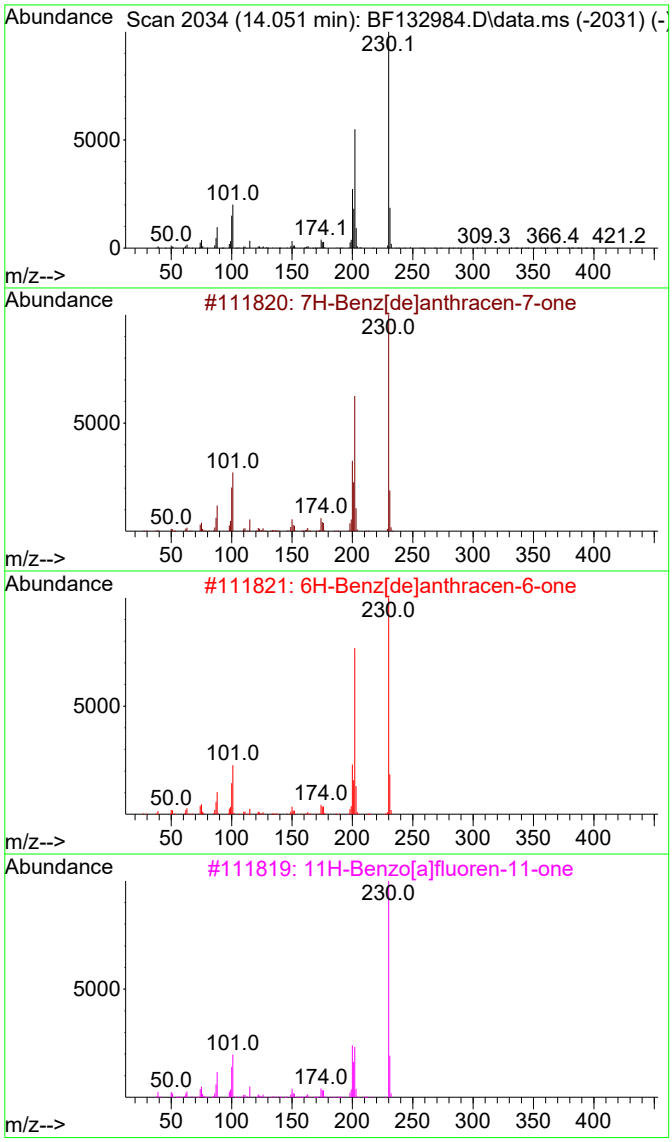
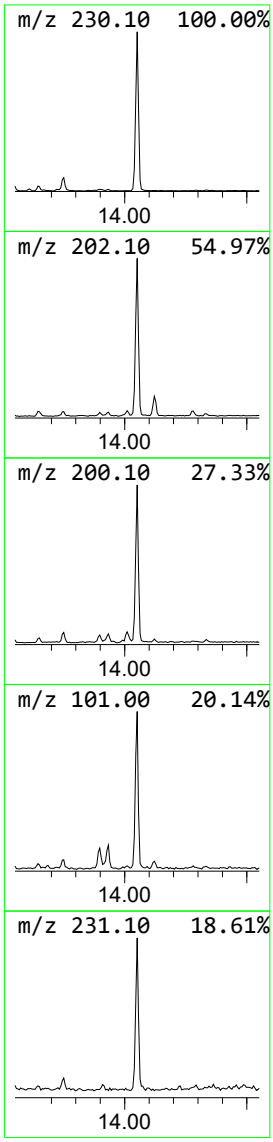
****

Peak Number 6 7H-Benz[de]anthracen-7-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.051	10.15 ng	880433	Chrysene-d12	13.910

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	98
3	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	95
4	1-Pyrenecarboxaldehyde	230	C17H10O	003029-19-4	68
5	o-Terphenyl	230	C18H14	000084-15-1	59





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

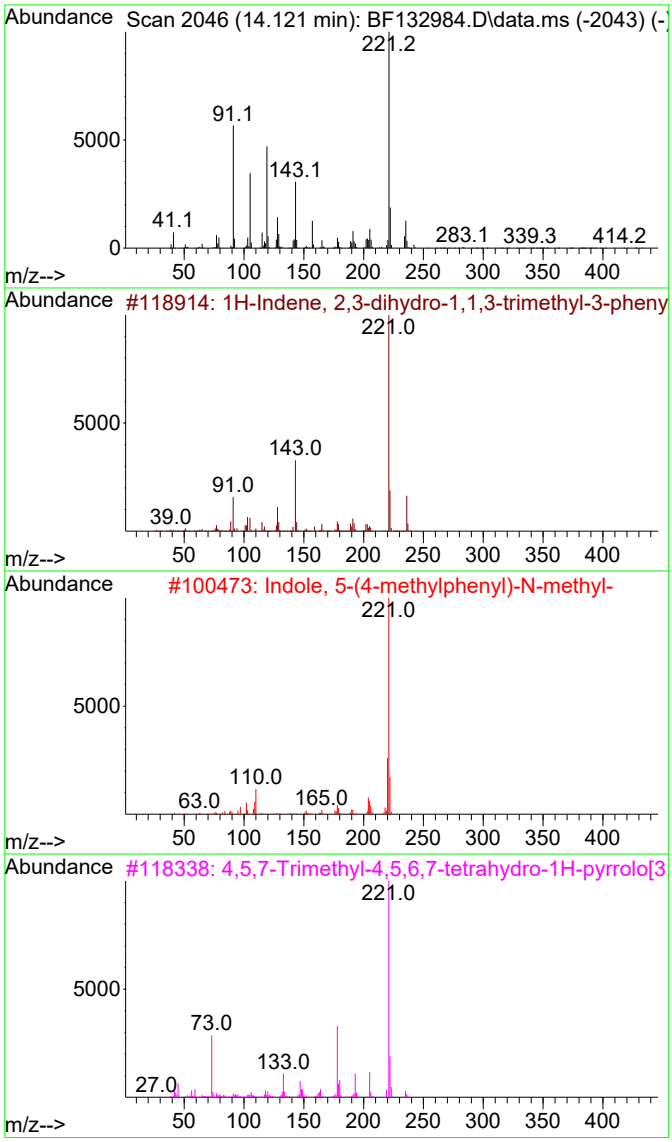
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

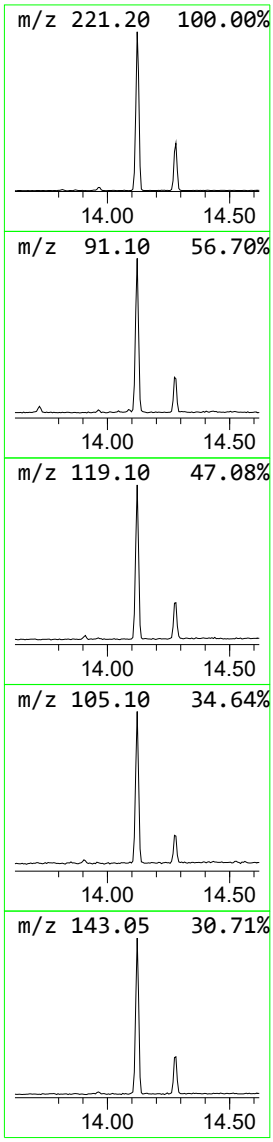
****

Peak Number 7 unknown14.121 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.121	28.83 ng	2500050	Chrysene-d12	13.910

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	Indole, 5-(4-methylphenyl)-N-met...	221	C16H15N	1000380-54-7	43
3	4,5,7-Trimethyl-4,5,6,7-tetrahyd...	236	C13H24N2Si	1000475-28-6	38
4	2-Mercapto-4,6-dimethylnicotinon...	236	C11H16N2SSi	1000332-43-1	38
5	1,3-Cyclohexanedione, 2-[2-[4-(4...	401	C22H28FN3O3	339310-26-8	38





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Instrument :
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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
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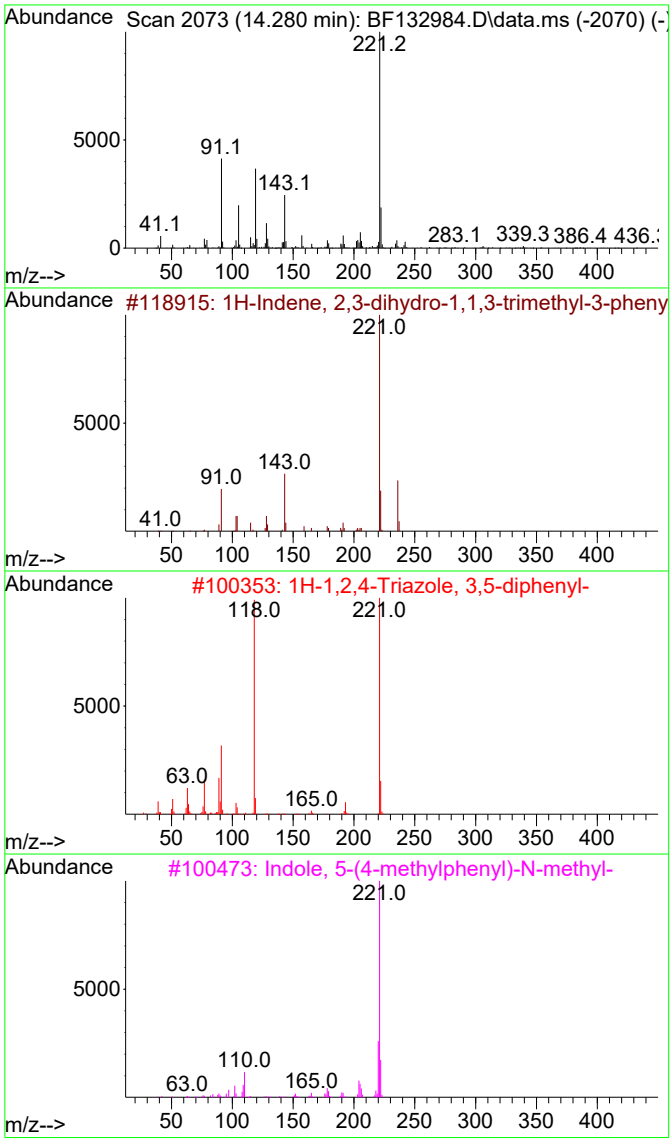
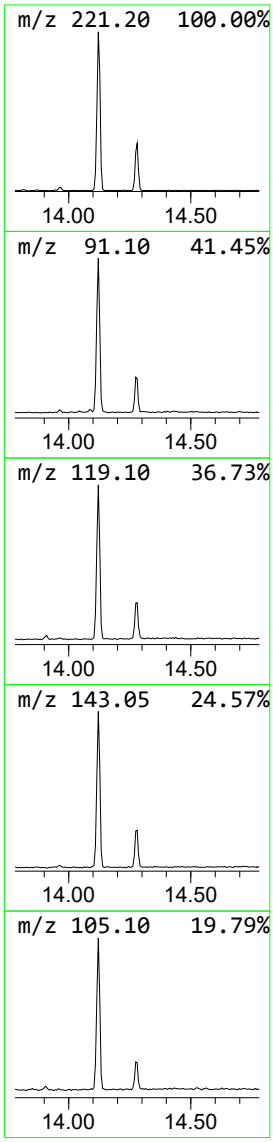
****

Peak Number 8 unknown14.280 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.280	7.14 ng	619390	Chrysene-d12	13.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	53
2	1H-1,2,4-Triazole, 3,5-diphenyl-	221	C14H11N3	002039-06-7	43
3	Indole, 5-(4-methylphenyl)-N-met...	221	C16H15N	1000380-54-7	43
4	2-Methyl-4,4-diphenyl-3,4-dihydr...	298	C21H18N2	1000300-40-0	38
5	1-(2-Hydroxy-4,5-dimethylphenyl)...	236	C13H20O2Si	1000484-73-7	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042123\
Data File : BF132984.D
Acq On : 21 Apr 2023 23:09
Operator : CG\JU
Sample : 02390-03 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPC-1WC-23-04-17

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

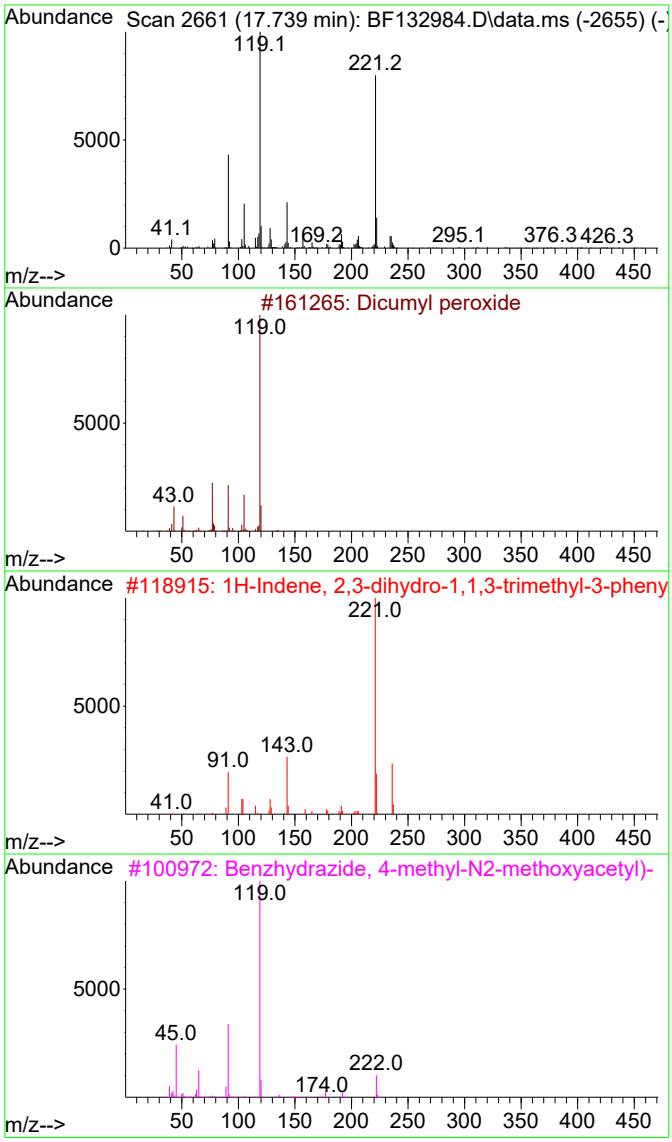
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

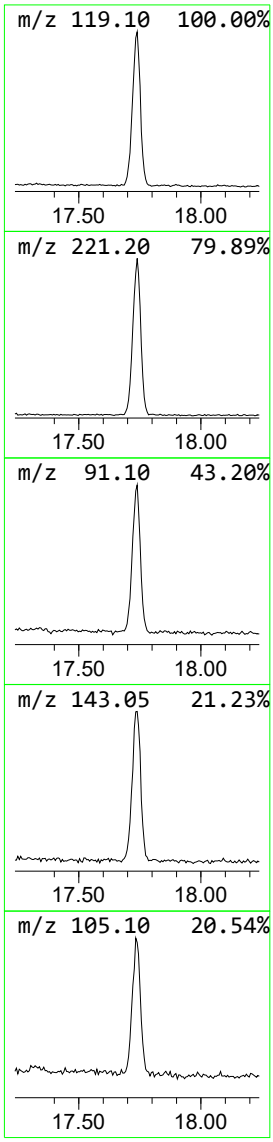
****

Peak Number 9 unknown17.739 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.739	29.46 ng	1037990	Perylene-d12	15.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dicumyl peroxide	270	C18H22O2	000080-43-3	35
2	1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	35
3	Benzhydrazide, 4-methyl-N2-metho...	222	C11H14N2O3	346456-58-4	27
4	Ethyl (4-methylbenzoyl)acetate	206	C12H14O3	027835-00-3	27
5	1H-1,2,3-Triazole, 4,5-diphenyl-	221	C14H11N3	005533-73-3	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042123\
Data File : BF132984.D
Acq On : 21 Apr 2023 23:09
Operator : CG\JU
Sample : 02390-03 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPC-1WC-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\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	4.940	8.4	ng	561833	1	6.751	1336070	20.0
1H-Indene, 2,3-...	10.880	3.2	ng	219155	4	11.269	1373500	20.0
n-Hexadecanoic ...	11.810	6.9	ng	472240	4	11.269	1373500	20.0
9,10-Anthracene...	12.086	3.1	ng	215526	4	11.269	1373500	20.0
Triphenylphosph...	14.010	7.0	ng	608195	5	13.910	1734320	20.0
7H-Benz[de]anth...	14.051	10.2	ng	880433	5	13.910	1734320	20.0
unknown14.121	14.121	28.8	ng	2500050	5	13.910	1734320	20.0
unknown14.280	14.280	7.1	ng	619390	5	13.910	1734320	20.0
unknown17.739	17.739	29.5	ng	1037990	6	15.339	704677	20.0