LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042123\
Data File : BF132981.D
Acq On : 21 Apr 2023 21:34
Operator : CG\JU
Sample : 02389-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPB-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: BF132981.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	8	18	rVB4	54474	100697	2.07%	0.187%
2	3.775	276	287	292	rBV	54821	86872	1.79%	0.162%
3	4.316	374	379	386	rBV	85933	107795	2.22%	0.201%
4	4.951	482	487	494	rVB	1056737	1478396	30.43%	2.750%
5	5.334	548	552	553	rBV	60951	55694	1.15%	0.104%
6	5.369	553	558	561	rVB	4730422	4775129	98.29%	8.884%
7	5.763	621	625	630	rBV	98012	88121	1.81%	0.164%
8	6.275	710	712	716	rBV3	47687	58892	1.21%	0.110%
9	6.387	726	731	734	rBV	4133062	4858270	100.00%	9.038%
10	6.575	760	763	765	rBV	81790	74240	1.53%	0.138%
11	6.751	789	793	796	rBV	1480643	1267401	26.09%	2.358%
12	6.816	800	804	811	rBV3	46657	82377	1.70%	0.153%
13	6.916	817	821	825	rVB	75192	70780	1.46%	0.132%
14	7.157	858	862	865	rBV2	59760	77544	1.60%	0.144%
15	7.316	882	889	894	rBV	3361682	3228424	66.45%	6.006%
16	7.357	894	896	900	rVB	80934	60033	1.24%	0.112%
17	7.975	998	1001	1003	rBV	95357	73220	1.51%	0.136%
18	8.034	1007	1011	1013	rVV	2078448	1617512	33.29%	3.009%
19	8.051	1013	1014	1017	rVV	178301	138246	2.85%	0.257%
20	8.104	1021	1023	1034	rVB4	29196	56308	1.16%	0.105%
21	8.192	1034	1038	1040	rBV3	50776	62930	1.30%	0.117%
22	8.745	1129	1132	1135	rVB	137387	106410	2.19%	0.198%
23	8.787	1135	1139	1146	rBV	68032	108961	2.24%	0.203%
24	8.845	1146	1149	1152	rVV2	71153	69763	1.44%	0.130%
25	9.110	1190	1194	1198	rVB	5168264	4846049	99.75%	9.015%
26	9.198	1203	1209	1213	rBV4	140862	202961	4.18%	0.378%
27	9.304	1223	1227	1230	rVB4	62531	82015	1.69%	0.153%
28	9.369	1235	1238	1242	rBV	66250	81280	1.67%	0.151%
29	9.445	1248	1251	1253	rBV2	75725	63582	1.31%	0.118%
30	9.498	1258	1260	1262	rBV2	80116	68088	1.40%	0.127%
31	9.645	1282	1285	1289	rBV	73405	87634	1.80%	0.163%
32	9.728	1297	1299	1303	rBV2	90180	80904	1.67%	0.151%
33	9.786	1303	1309	1312	rBV	1946236	1621711	33.38%	3.017%
34	9.816	1312	1314	1317	rBV	233660	188869	3.89%	0.351%
35	9.986	1341	1343	1346	rVB	142444	118937	2.45%	0.221%
36	10.198	1376	1379	1382	rBV2	100034	108771	2.24%	0.202%

LSC Area Percent Report

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	10.328	1399	1401	1405	rBV	136811	114642	2.36%	0.213%
38	10.422	1414	1417	1419	rBV	630589	647204	13.32%	1.204%
39	10.498	1426	1430	1434	rVB	550419	492884	10.15%	0.917%
40	10.575	1439	1443	1446	rBV	2613119	2331337	47.99%	4.337%
41	10.616	1446	1450	1453	rVB2	160328	153655	3.16%	0.286%
42	10.698	1462	1464	1465	rBV2	117863	95471	1.97%	0.178%
43	10.880	1492	1495	1498	rBV2	276451	235924	4.86%	0.439%
44	11.069	1525	1527	1531	rBV	133981	142919	2.94%	0.266%
45	11.269	1558	1561	1563	rBV	1425426	1277884	26.30%	2.377%
46	11.292	1563	1565	1568	rVV	1812089	1377506	28.35%	2.563%
47	11.339	1571	1573	1576	rVB	473708	380267	7.83%	0.707%
48	11.492	1597	1599	1602	rBV	208974	177949	3.66%	0.331%
49	11.810	1648	1653	1657	rBV2	572223	844635	17.39%	1.571%
50	11.880	1662	1665	1671	rVB4	484648	714591	14.71%	1.329%
51	12.086	1698	1700	1702	rBV	633333	430965	8.87%	0.802%
52	12.486	1764	1768	1771	rBV	2397201	2214757	45.59%	4.120%
53	12.710	1802	1806	1811	rVB	2026331	2230910	45.92%	4.150%
54	12.863	1828	1832	1836	rBV	3394824	3150105	64.84%	5.860%
55	13.910	2006	2010	2013	rBV3	1878992	2396670	49.33%	4.459%
56	13.939	2013	2015	2017	rVB	1162740	838325	17.26%	1.560%
57	14.057	2032	2035	2038	rVB	1256443	1099160	22.62%	2.045%
58	14.127	2044	2047	2053	rVB	2944839	2913101	59.96%	5.419%
59	14.280	2071	2073	2080	rVB2	739025	829031	17.06%	1.542%
60	15.233	2232	2235	2240	rVB2	882708	1141705	23.50%	2.124%
61	17.745	2658	2662	2672	rVB	565182	1266018	26.06%	2.355%

Sum of corrected areas: 53752431

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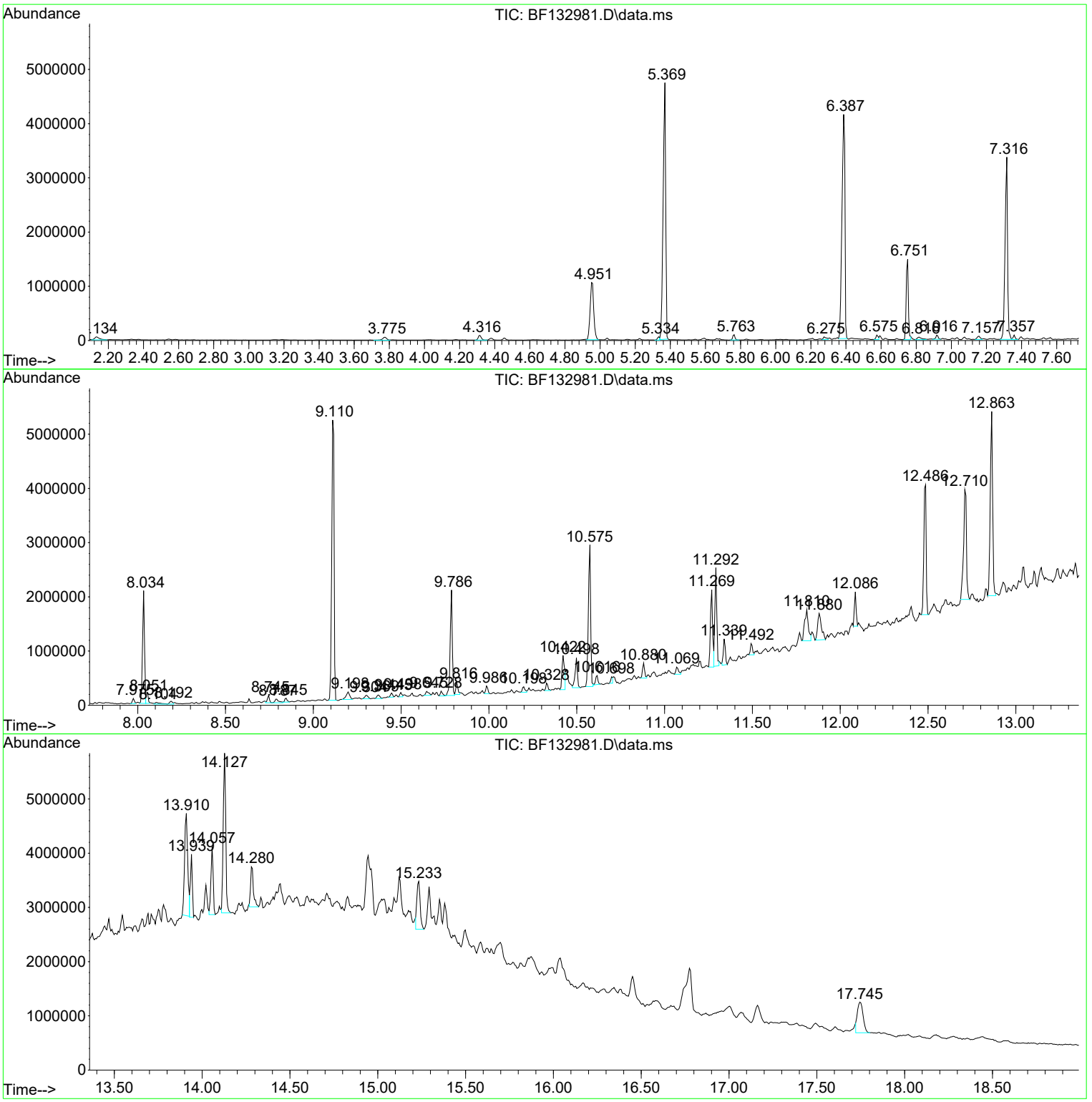
ClientSampleId :
SPB-1WC-23-04-17

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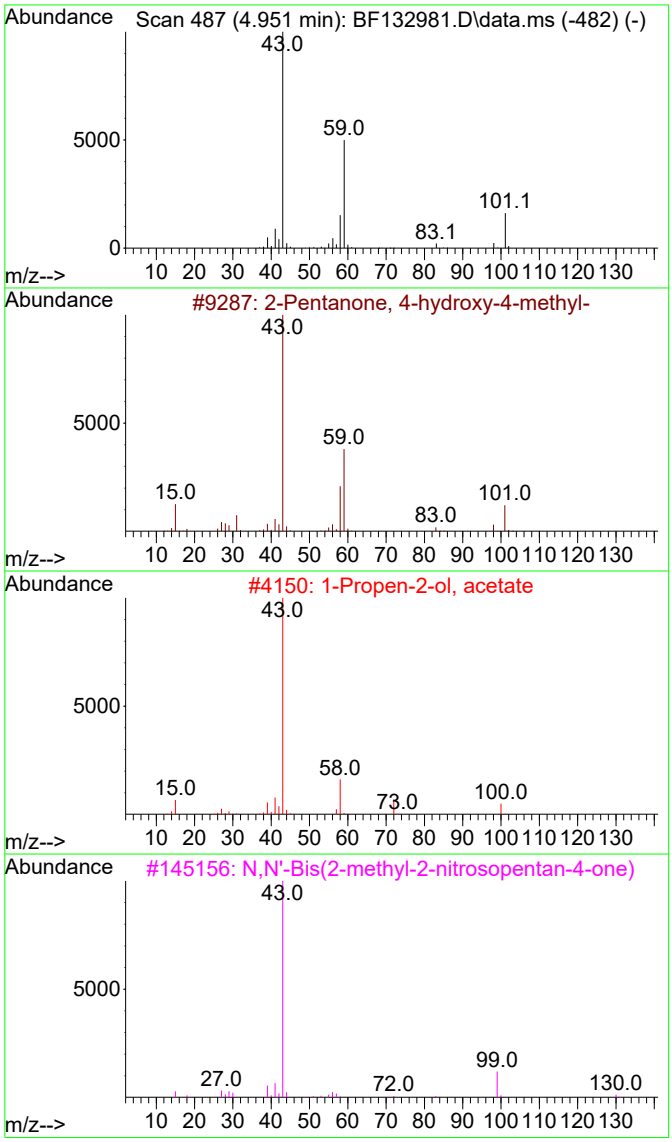
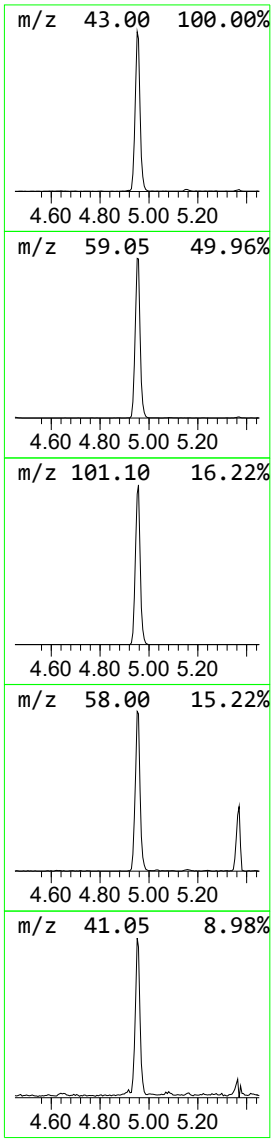
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.951	23.33 ng	1478400	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	59
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3	N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	9
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	7





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Acq On : 21 Apr 2023 21:34
Operator : CG\JU
Sample : 02389-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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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
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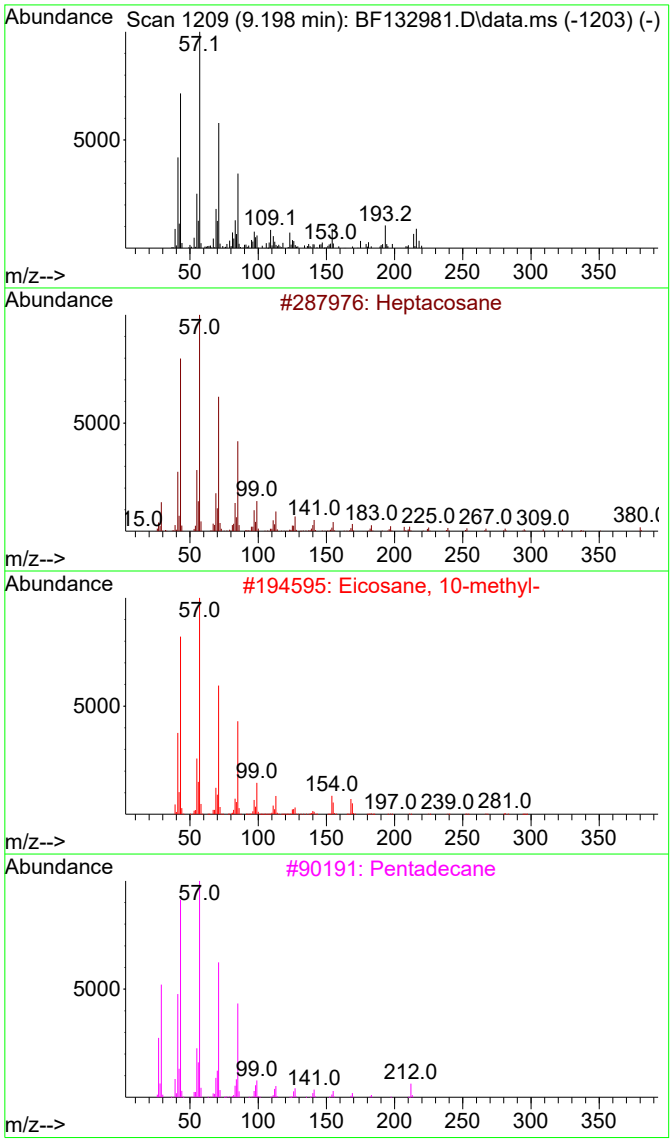
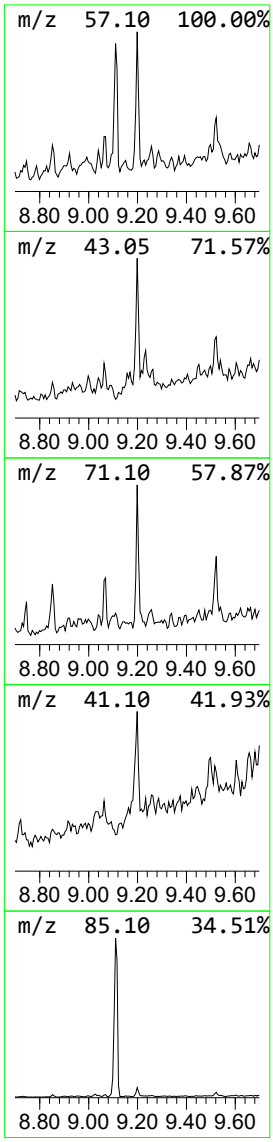
****

Peak Number 2 Heptacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.198	2.50 ng	202961	Acenaphthene-d10	9.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	58
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	58
3	Pentadecane	212	C15H32	000629-62-9	58
4	Tridecane	184	C13H28	000629-50-5	58
5	Heptadecane	240	C17H36	000629-78-7	53





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ClientSampleId :
SPB-1WC-23-04-17

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

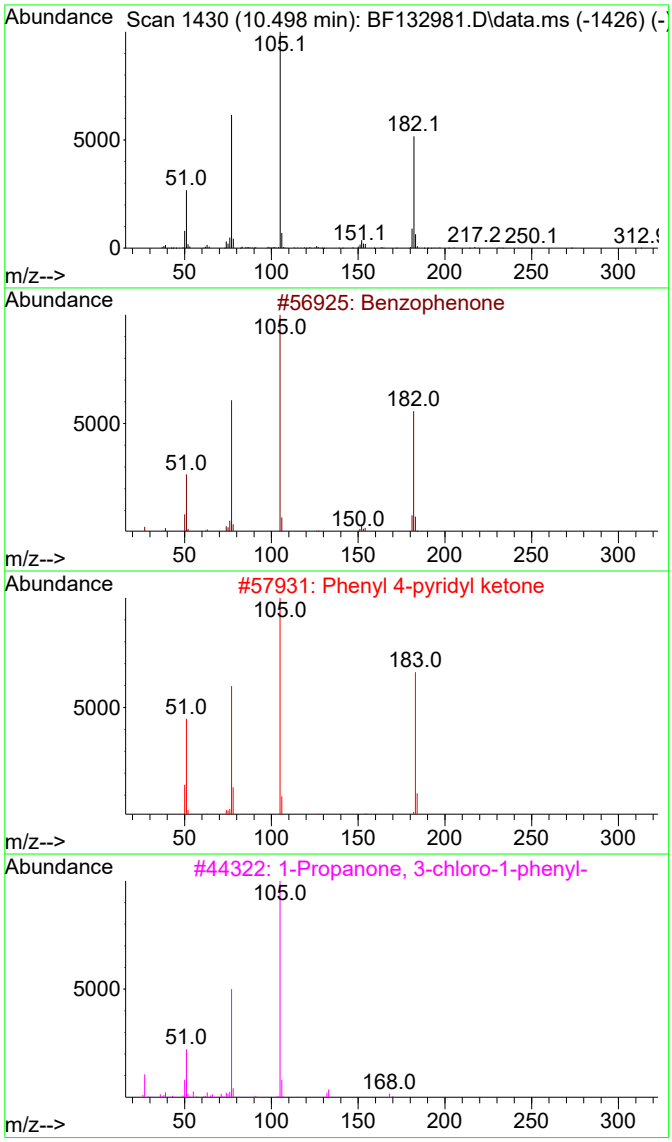
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

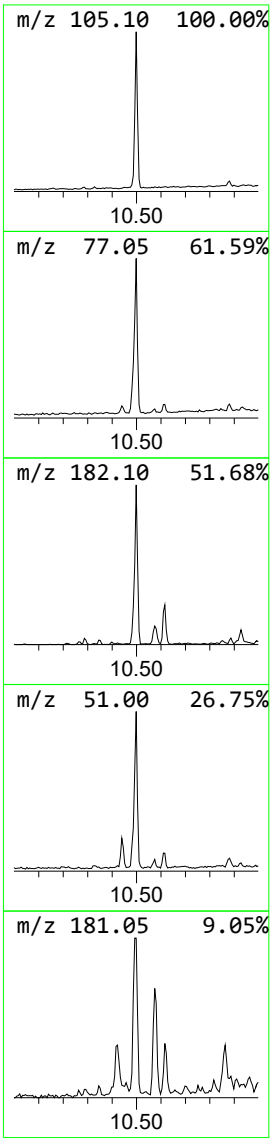
****

Peak Number 3 Benzophenone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.498	6.08 ng	492884	Acenaphthene-d10	9.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	53
3	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
4	acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	47
5	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47





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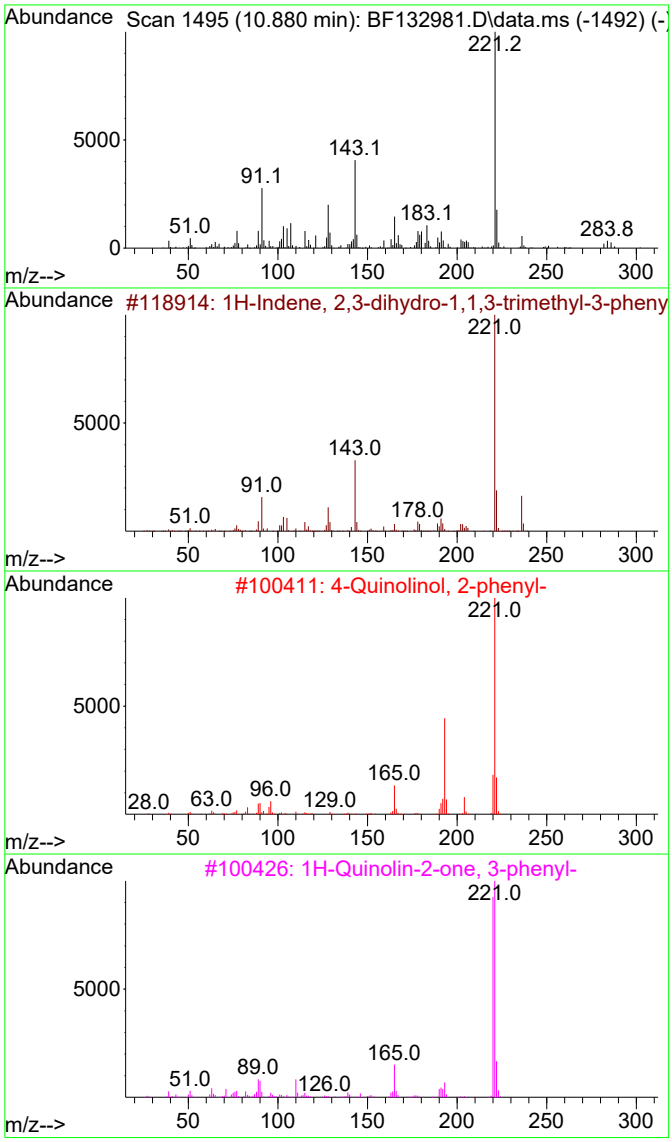
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

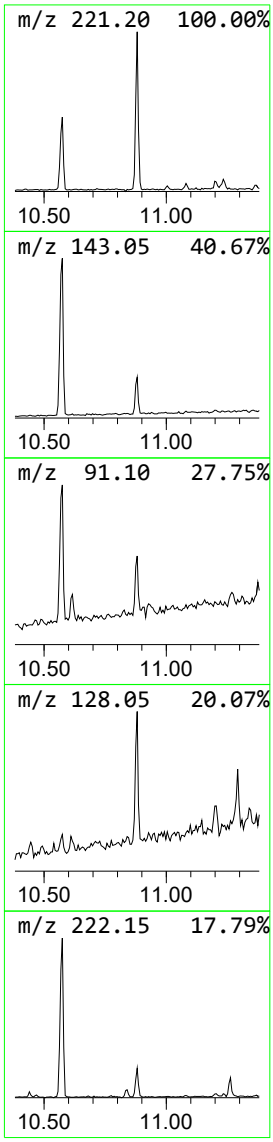
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1H-Indene, 2,3-dihydro-1,1,... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.881	3.69 ng	235924	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	72
2	4-Quinolinol, 2-phenyl-	221	C15H11NO	001144-20-3	43
3	1H-Quinolin-2-one, 3-phenyl-	221	C15H11NO	038035-81-3	38
4	1H-1,2,3-Triazole, 4,5-diphenyl-	221	C14H11N3	005533-73-3	38
5	Benzene, 1-(1-hydroxyheptyl)-3-[...	390	C25H42O3	1000196-54-9	38





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

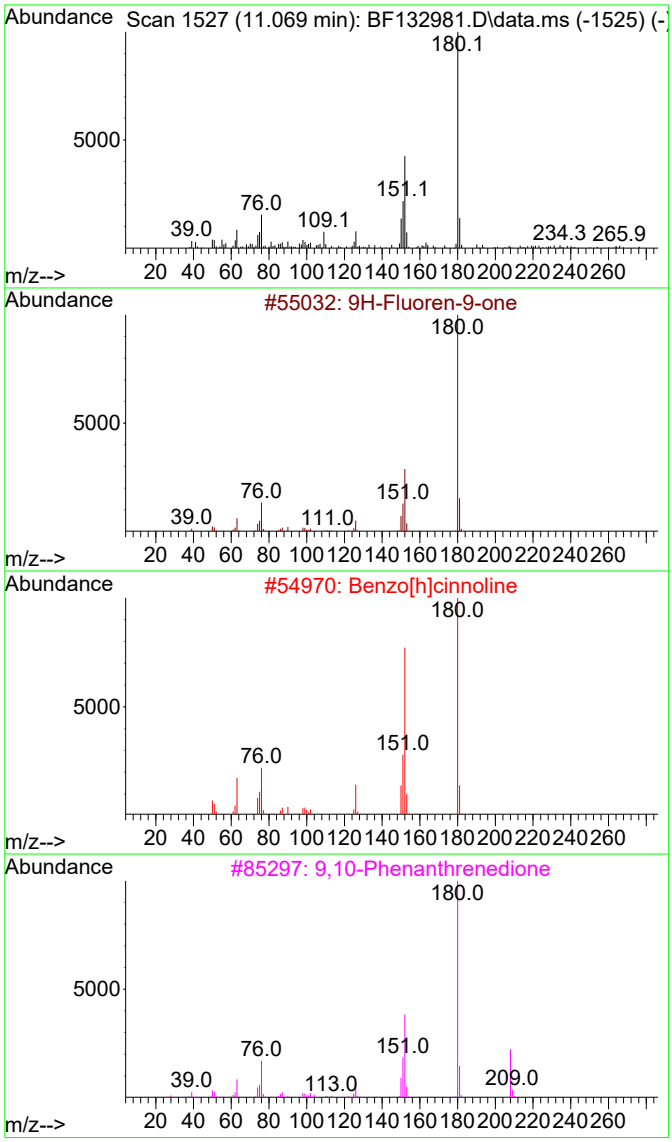
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

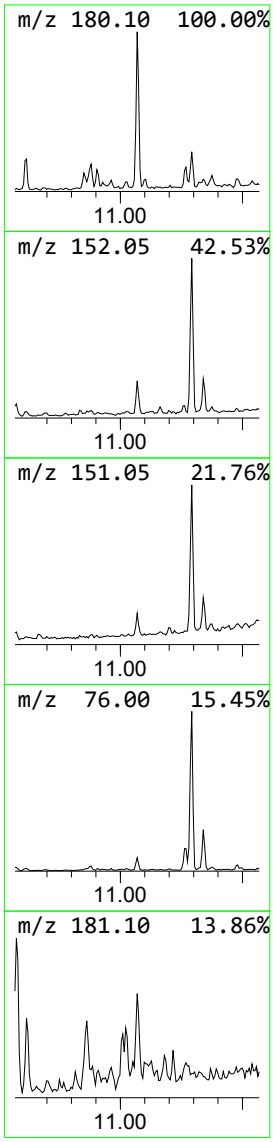
****

Peak Number 5 9H-Fluoren-9-one Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.069	2.24 ng	142919	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9H-Fluoren-9-one	180	C13H8O	000486-25-9	96
2	Benzo[h]cinnoline	180	C12H8N2	000230-31-9	91
3	9,10-Phenanthrenedione	208	C14H8O2	000084-11-7	91
4	1H-Phenalen-1-one	180	C13H8O	000548-39-0	64
5	Diphenic anhydride	224	C14H8O3	006050-13-1	62





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

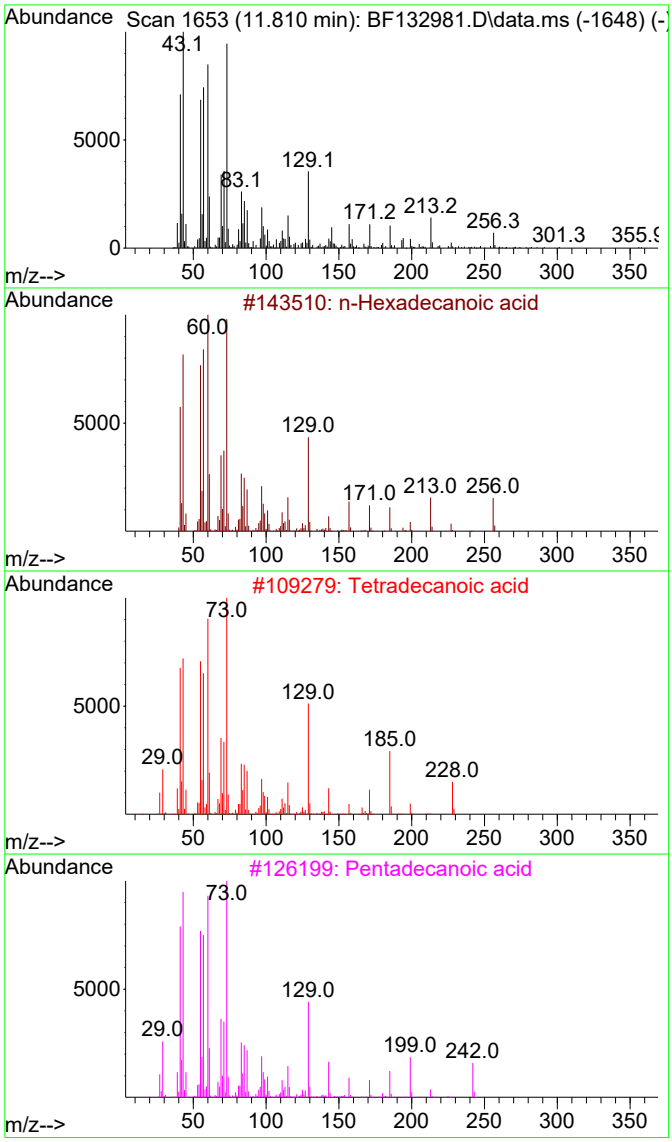
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

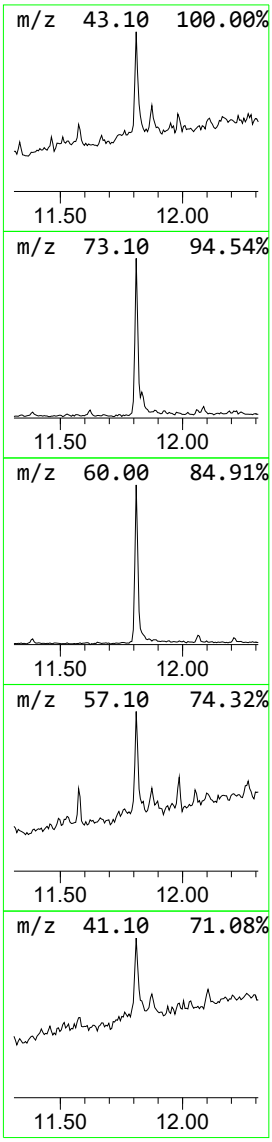
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.810	13.22 ng	844635	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Octadecanoic acid	284	C18H36O2	000057-11-4	81
5	Tridecanoic acid	214	C13H26O2	000638-53-9	80





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Operator : CG\JU
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ALS Vial : 18 Sample Multiplier: 1

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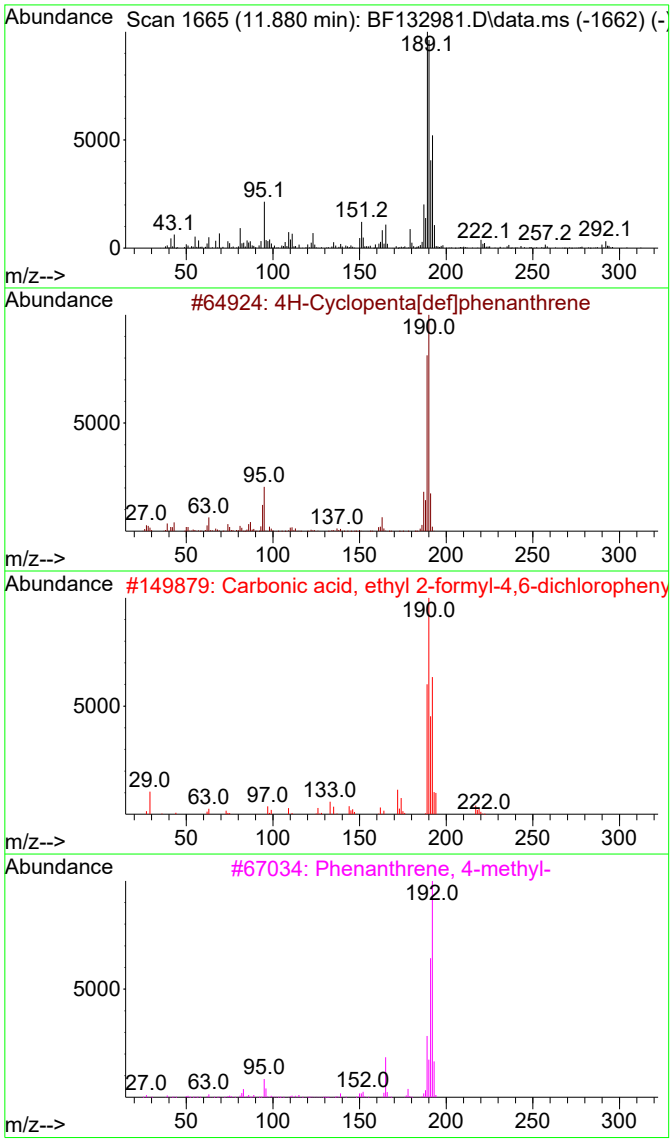
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

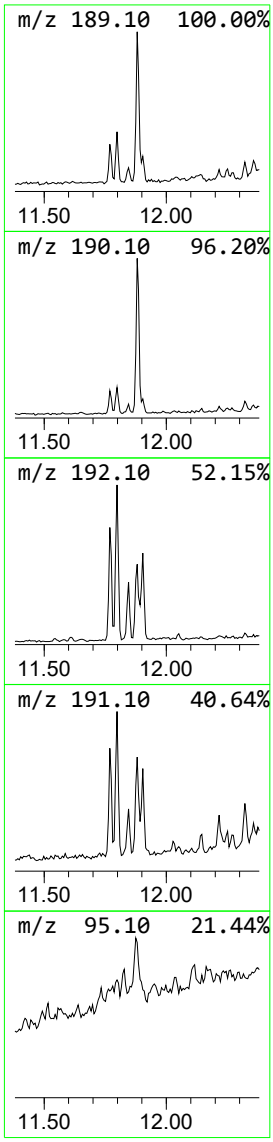
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.880	11.18 ng	714591	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	50
3	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	38
4	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	30
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	25





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Data File : BF132981.D
Acq On : 21 Apr 2023 21:34
Operator : CG\JU
Sample : 02389-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

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

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

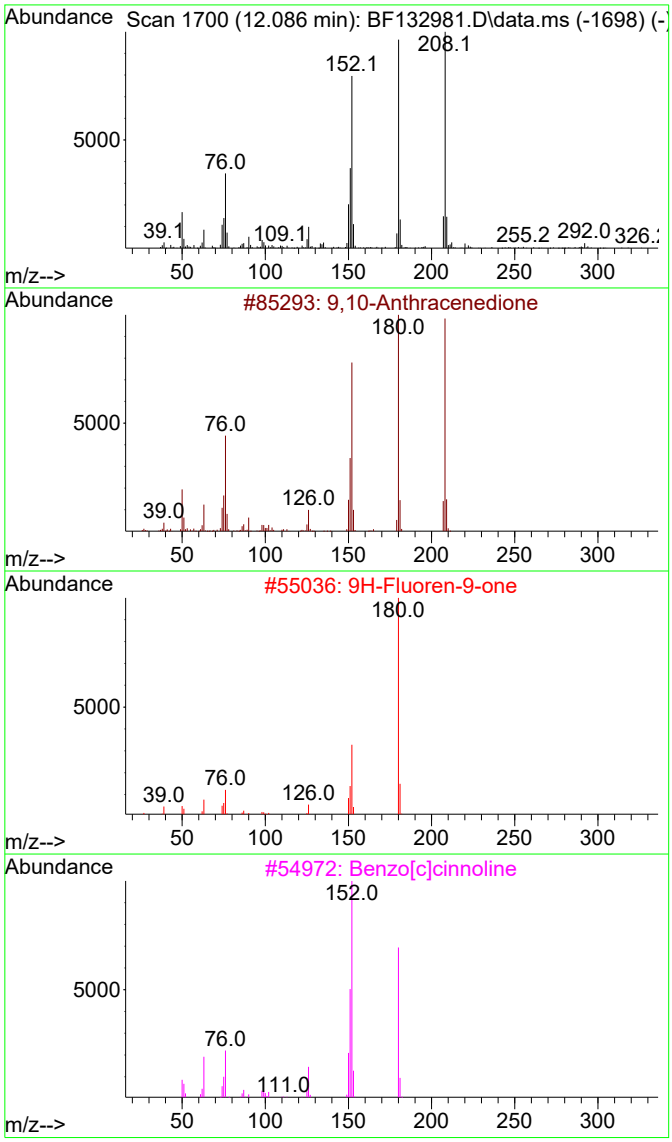
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

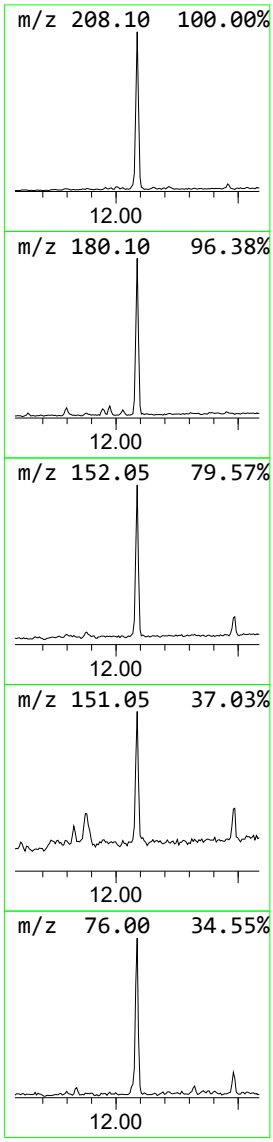
****

Peak Number 8 9,10-Anthracenedione Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.086	6.74 ng	430965	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione	208	C14H8O2	000084-65-1	98
2	9H-Fluoren-9-one	180	C13H8O	000486-25-9	83
3	Benzo[c]cinnoline	180	C12H8N2	000230-17-1	64
4	1H-Phenalen-1-one	180	C13H8O	000548-39-0	64
5	2-(Dicyanomethylene)indene-1,3-d...	208	C12H4N2O2	016954-74-8	58





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Operator : CG\JU
Sample : 02389-03
Misc :
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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

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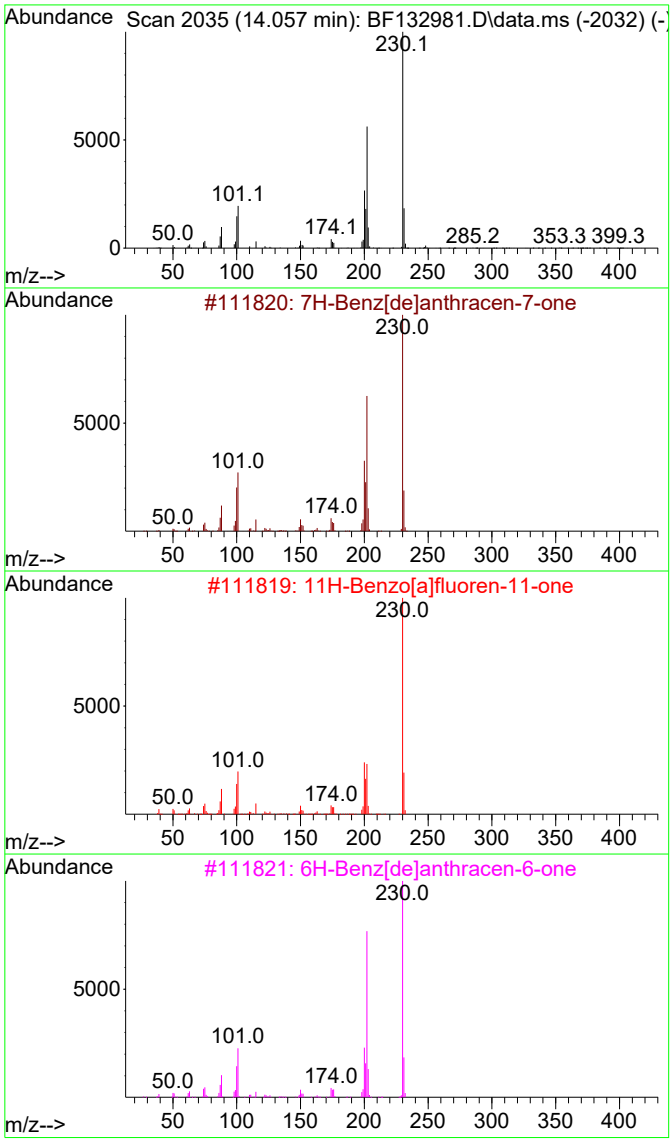
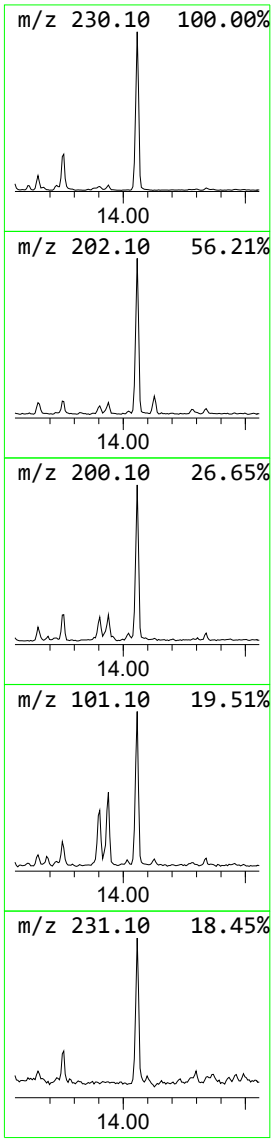
Peak Number 9 7H-Benz[de]anthracen-7-one Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.057	9.17 ng	1099160	Chrysene-d12	13.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	97
2	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	96
3	6H-Benz[de]anthracen-6-one	230	C17H10O	080252-14-8	96
4	Pyrene	202	C16H10	000129-00-0	86
5	4-Pyrenecarbaldehyde	230	C17H10O	022245-51-8	68





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Operator : CG\JU
Sample : 02389-03
Misc :
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Instrument :
BNA_F
ClientSampleId :
SPB-1WC-23-04-17

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
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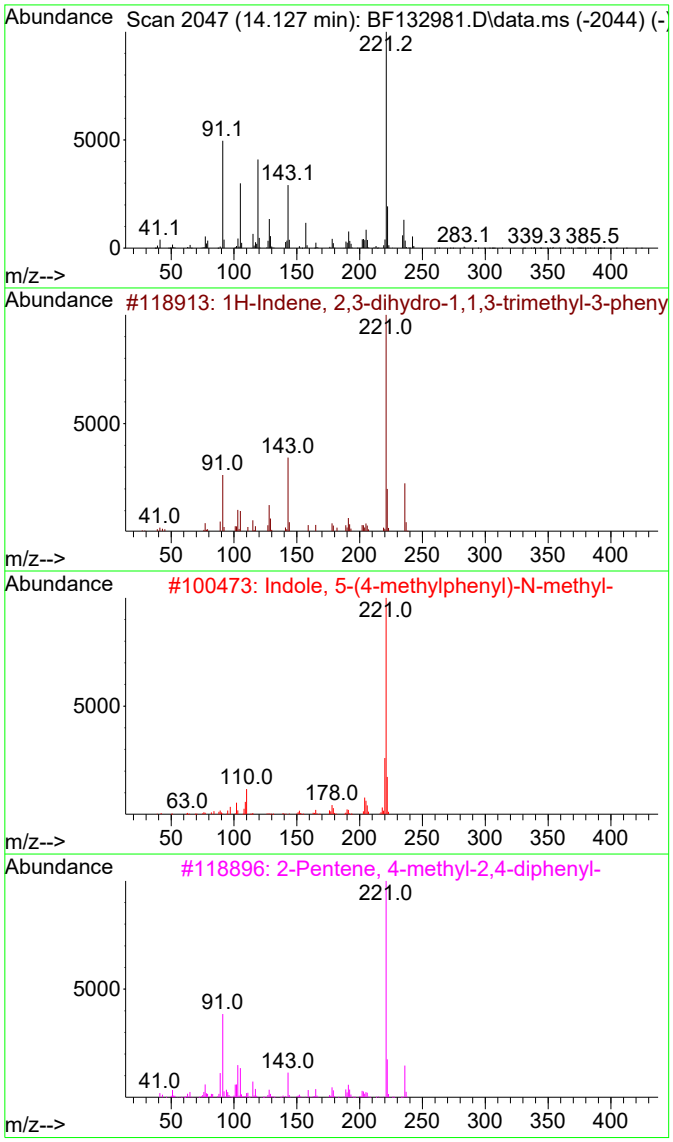
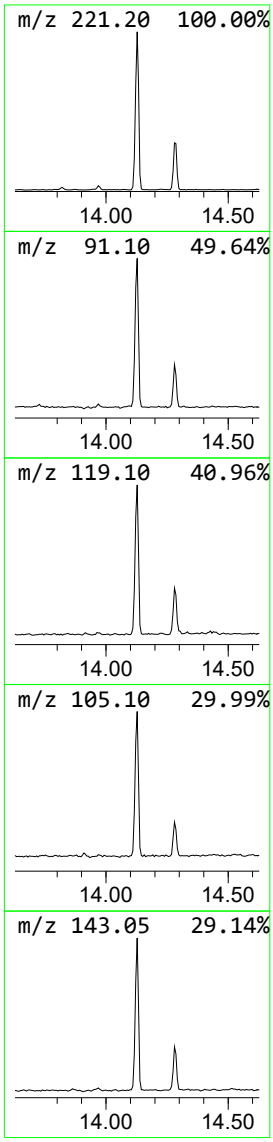
Peak Number 10 unknown14.127 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.127	24.31 ng	2913100	Chrysene-d12	13.916

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	2-Pentene, 4-methyl-2,4-diphenyl-	236	C18H20	006258-73-7	40
4	Oxazole, 2,5-diphenyl-	221	C15H11NO	000092-71-7	38
5	4-Hydroxy-beta-phenylcinnamonitrile	221	C15H11NO	016281-90-6	38





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Misc :
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
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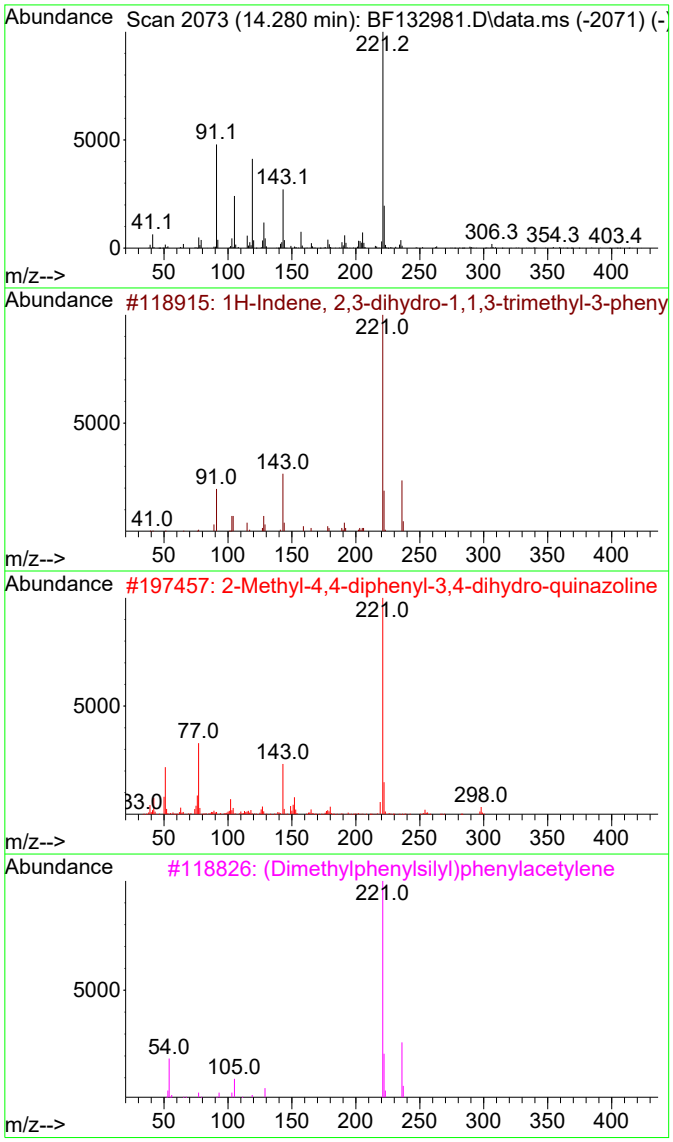
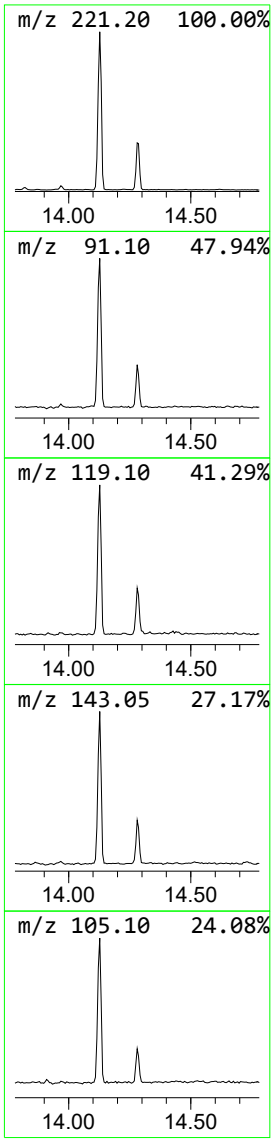
Peak Number 11 unknown14.280 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.280	6.92 ng	829031	Chrysene-d12	13.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	50
2	2-Methyl-4,4-diphenyl-3,4-dihydr...	298	C21H18N2	1000300-40-0	47
3	(Dimethylphenylsilyl)phenylacety...	236	C16H16Si	1000434-31-1	47
4	1-(2-Hydroxy-4,5-dimethylphenyl)...	236	C13H20O2Si	1000484-73-7	38
5	Boron, diethyl(5-ethyl-4,6-nonan...	250	C15H31BN2	136705-03-8	35





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Operator : CG\JU
Sample : 02389-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPB-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
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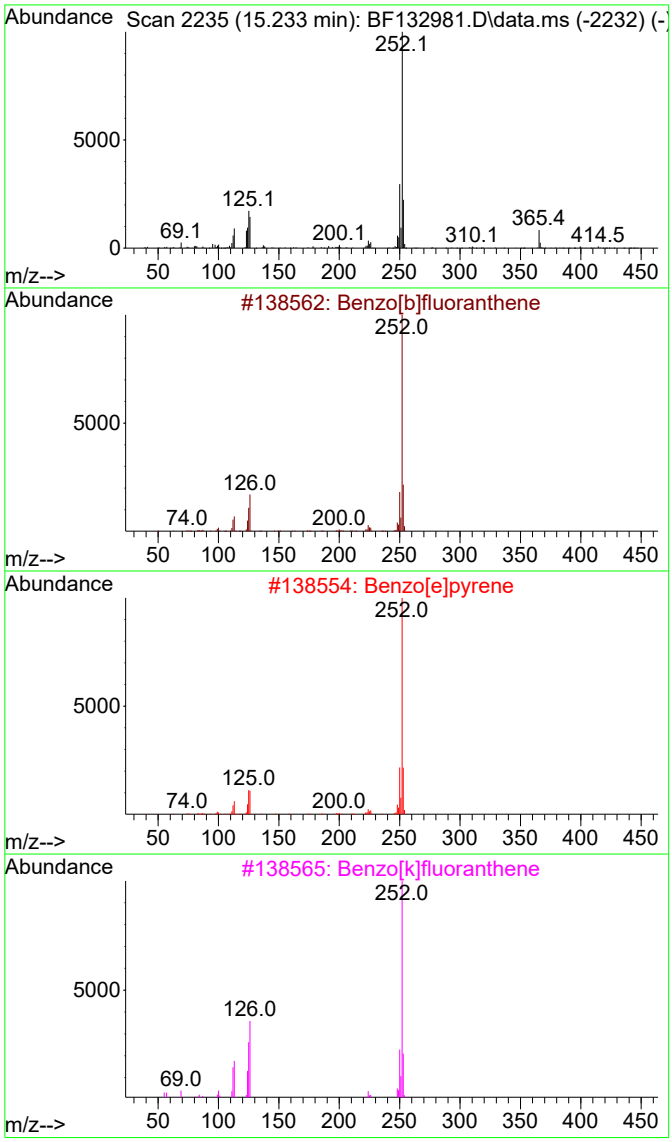
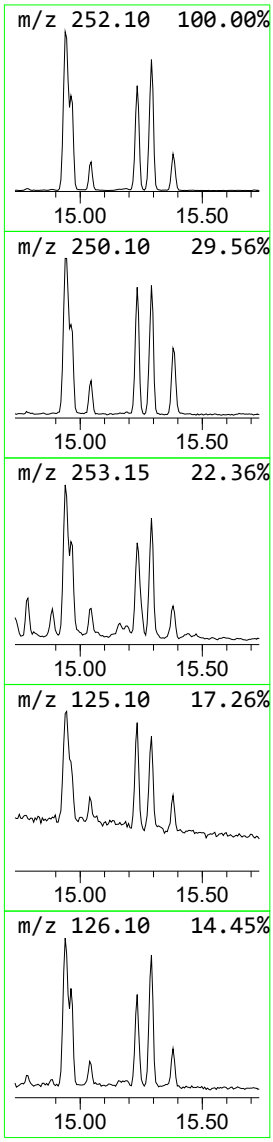
Peak Number 12 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.233	20.00 ng	1141710	Perylene-d12	15.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]fluoranthene	252	C20H12	000205-99-2	98
2	Benzo[e]pyrene	252	C20H12	000192-97-2	97
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
4	Perylene	252	C20H12	000198-55-0	94
5	Benzo[a]pyrene	252	C20H12	000050-32-8	92





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Operator : CG\JU
Sample : 02389-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPB-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
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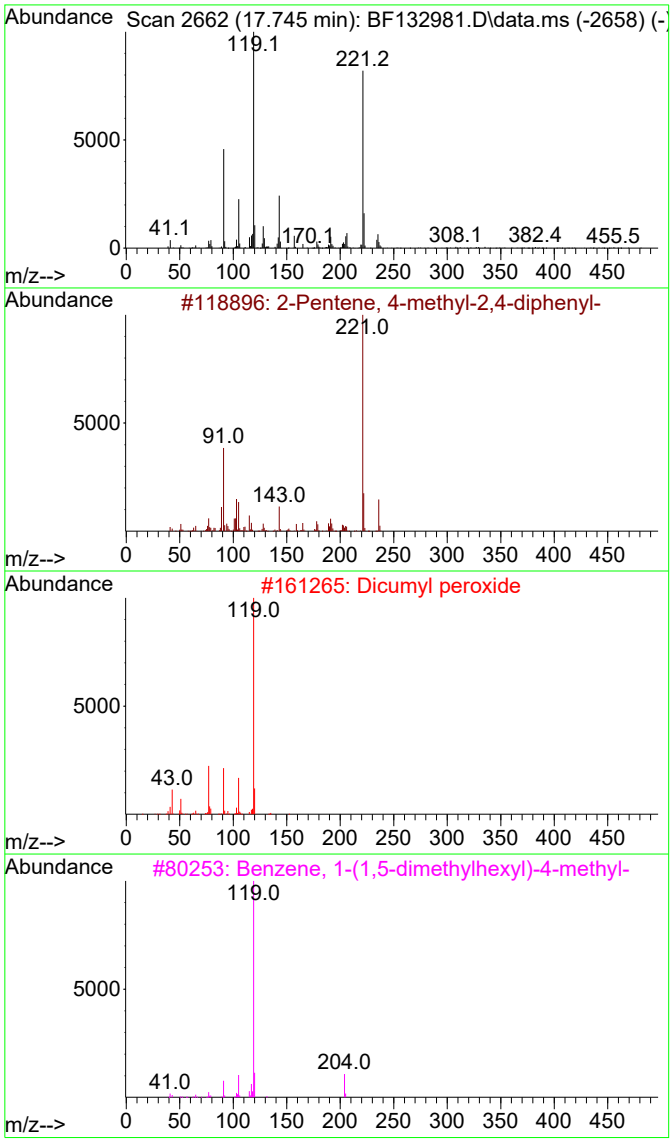
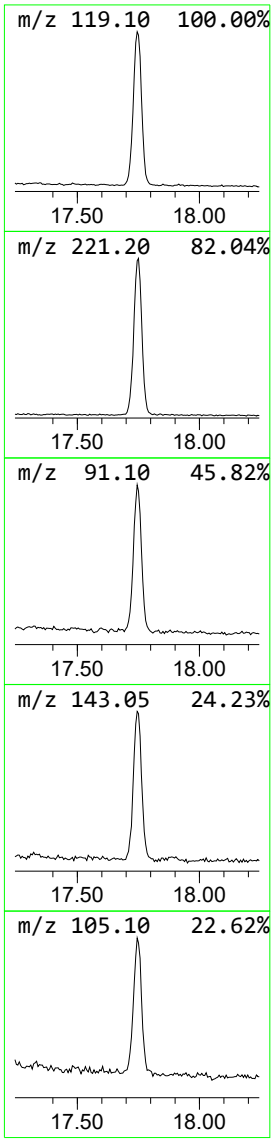
Peak Number 13 unknown17.745 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.745	22.18 ng	1266020	Perylene-d12	15.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, 4-methyl-2,4-diphenyl-	236	C18H20	006258-73-7	43
2	Dicumyl peroxide	270	C18H22O2	000080-43-3	35
3	Benzene, 1-(1,5-dimethylhexyl)-4...	204	C15H24	001461-02-5	27
4	Ethyl (4-methylbenzoyl)acetate	206	C12H14O3	027835-00-3	27
5	2,4-Diphenyl-4-methyl-1-pentene	236	C18H20	1000111-58-0	25





Tentatively Identified Compound (LSC) summary

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Data File : BF132981.D
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Operator : CG\JU
Sample : 02389-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPB-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-...	4.951	23.3	ng	1478400	1	6.751	1267400	20.0
Heptacosane	9.198	2.5	ng	202961	3	9.786	1621710	20.0
Benzophenone	10.498	6.1	ng	492884	3	9.786	1621710	20.0
1H-Indene, 2,3-...	10.881	3.7	ng	235924	4	11.269	1277880	20.0
9H-Fluoren-9-one	11.069	2.2	ng	142919	4	11.269	1277880	20.0
n-Hexadecanoic ...	11.810	13.2	ng	844635	4	11.269	1277880	20.0
4H-Cyclopenta[d...	11.880	11.2	ng	714591	4	11.269	1277880	20.0
9,10-Anthracene...	12.086	6.7	ng	430965	4	11.269	1277880	20.0
7H-Benz[de]anth...	14.057	9.2	ng	1099160	5	13.916	2396670	20.0
unknown14.127	14.127	24.3	ng	2913100	5	13.916	2396670	20.0
unknown14.280	14.280	6.9	ng	829031	5	13.916	2396670	20.0
Benzo[e]pyrene	15.233	20.0	ng	1141710	6	15.351	1141710	20.0
unknown17.745	17.745	22.2	ng	1266020	6	15.351	1141710	20.0