LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030923\
Data File : BF132716.D
Acq On : 09 Mar 2023 14:03
Operator : CG\JU
Sample : 01834-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-10

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-BF022223.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132716.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.210	441	446	457	rVB	1716963	2158718	48.70%	5.861%
2	5.610	510	514	524	rBV	4182784	4086474	92.19%	11.095%
3	6.610	680	684	695	rBV	3801415	4080170	92.04%	11.078%
4	6.981	743	747	750	rBV	1301243	1048599	23.66%	2.847%
5	7.545	838	843	846	rBV	3042093	2636746	59.48%	7.159%
6	8.263	962	965	968	rBV	1742526	1388334	31.32%	3.770%
7	8.975	1083	1086	1090	rBV	80213	69915	1.58%	0.190%
8	9.075	1101	1103	1107	rVB	117664	97001	2.19%	0.263%
9	9.339	1144	1148	1151	rBV	5582908	4432859	100.00%	12.036%
10	9.610	1189	1194	1198	rBV2	58272	80802	1.82%	0.219%
11	9.681	1202	1206	1208	rBV	94962	91863	2.07%	0.249%
12	9.886	1237	1241	1245	rBV2	93860	90175	2.03%	0.245%
13	10.028	1261	1265	1268	rVV	1587629	1432811	32.32%	3.890%
14	10.057	1268	1270	1273	rVB	80290	60123	1.36%	0.163%
15	10.222	1295	1298	1302	rVB2	53183	61858	1.40%	0.168%
16	10.339	1314	1318	1320	rBV3	48804	53144	1.20%	0.144%
17	10.433	1329	1334	1339	rVB6	38033	75778	1.71%	0.206%
18	10.575	1355	1358	1363	rVB	117709	111144	2.51%	0.302%
19	10.739	1382	1386	1389	rVB	305149	263107	5.94%	0.714%
20	10.816	1395	1399	1403	rBV	2586808	2523634	56.93%	6.852%
21	10.933	1413	1419	1426	rVB7	31403	78544	1.77%	0.213%
22	11.122	1446	1451	1454	rBV2	42163	57937	1.31%	0.157%
23	11.522	1515	1519	1521	rBV	1507758	1276802	28.80%	3.467%
24	11.545	1521	1523	1526	rVB	368471	280633	6.33%	0.762%
25	11.598	1526	1532	1534	rBV	76223	97676	2.20%	0.265%
26	12.033	1601	1606	1608	rBV2	287438	335614	7.57%	0.911%
27	12.051	1608	1609	1615	rVB2	144930	113458	2.56%	0.308%
28	12.139	1620	1624	1626	rVV2	164523	186997	4.22%	0.508%
29	12.157	1626	1627	1631	rVB	77847	59002	1.33%	0.160%
30	12.574	1695	1698	1701	rBV	75462	78842	1.78%	0.214%
31	12.663	1711	1713	1722	rVB7	37634	82117	1.85%	0.223%
32	12.739	1723	1726	1730	rBV	426153	398280	8.98%	1.081%
33	12.974	1759	1766	1771	rBV	583618	589630	13.30%	1.601%
34	13.110	1785	1789	1792	rBV	3731424	3169420	71.50%	8.605%
35	13.192	1799	1803	1807	rBV3	45174	68767	1.55%	0.187%
36	13.304	1815	1822	1824	rBV	106703	172630	3.89%	0.469%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030923\
Data File : BF132716.D
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Operator : CG\JU
Sample : 01834-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-10

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-BF022223.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.369	1830	1833	1836	rVB	84513	64287	1.45%	0.175%
38	13.410	1837	1840	1843	rVB2	78765	67012	1.51%	0.182%
39	13.533	1858	1861	1864	rBV	69826	66633	1.50%	0.181%
40	13.998	1935	1940	1952	rBV4	353412	603588	13.62%	1.639%
41	14.139	1961	1964	1966	rBV	100066	86490	1.95%	0.235%
42	14.180	1966	1971	1974	rVV2	1368496	1413217	31.88%	3.837%
43	14.204	1974	1975	1981	rVB	270602	205302	4.63%	0.557%
44	14.268	1982	1986	1989	rVV	455125	433913	9.79%	1.178%
45	14.321	1992	1995	2003	rVB4	52491	85653	1.93%	0.233%
46	14.568	2035	2037	2040	rVB	85899	70506	1.59%	0.191%
47	15.263	2151	2155	2158	rBV	223437	324503	7.32%	0.881%
48	15.592	2207	2211	2216	rVB	142443	196164	4.43%	0.533%
49	15.657	2218	2222	2227	rBV	232389	292347	6.59%	0.794%
50	15.727	2229	2234	2238	rBV	766332	1031491	23.27%	2.801%

Sum of corrected areas: 36830710

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BNA_F
ClientSampleId :
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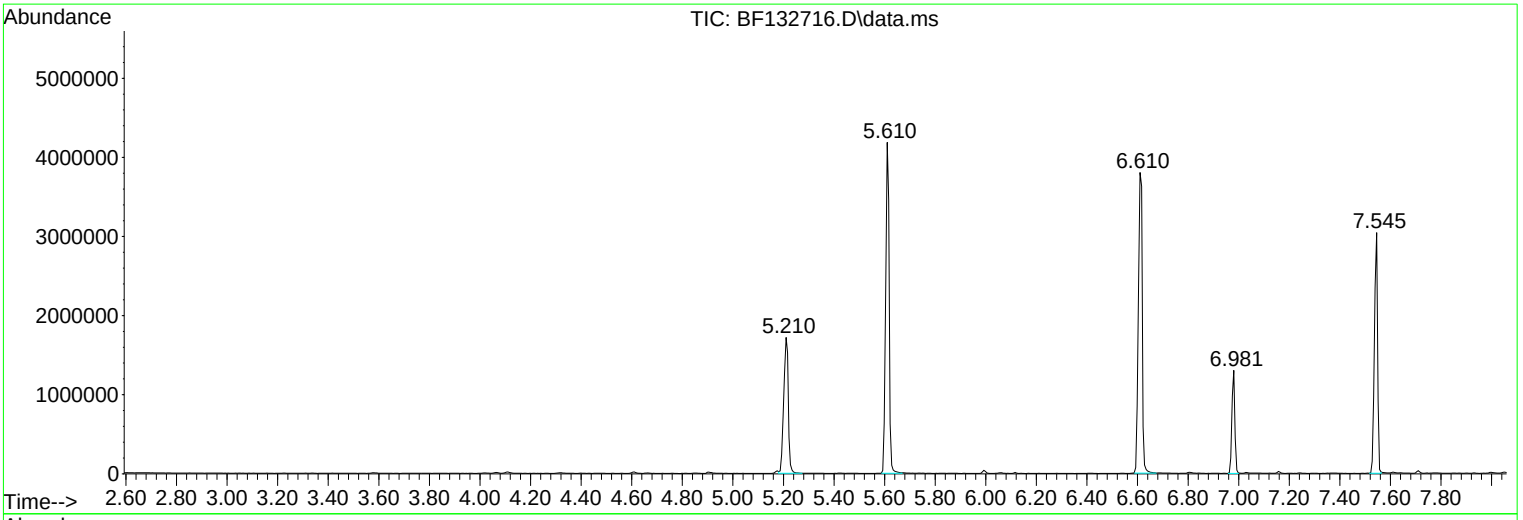
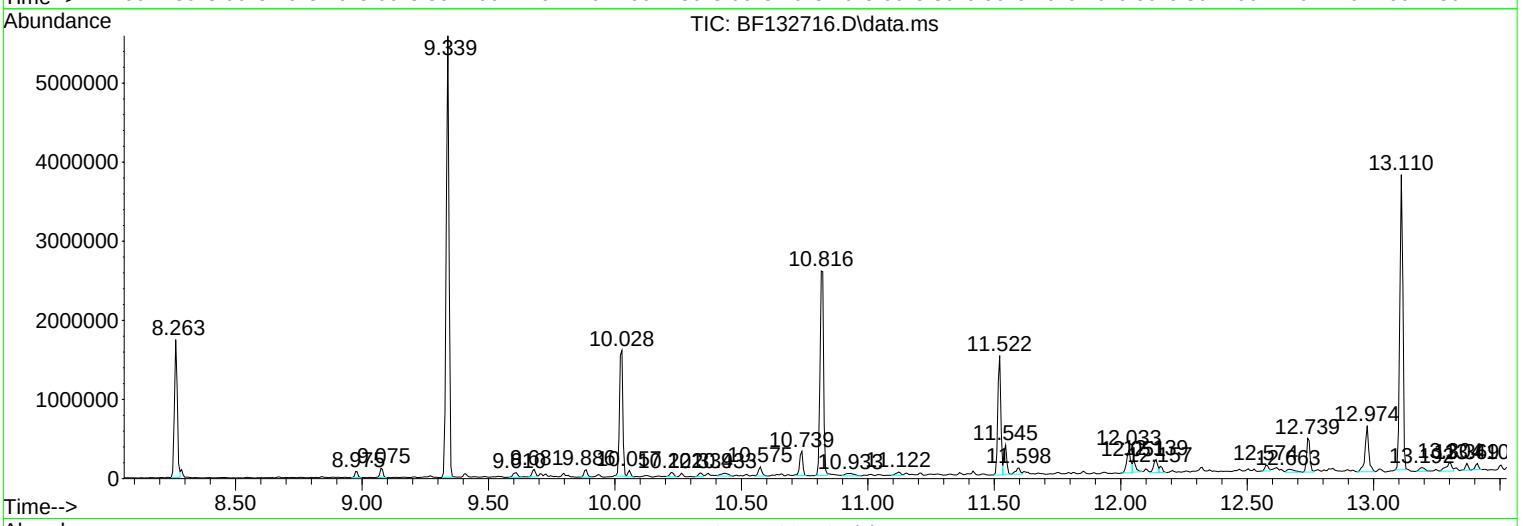
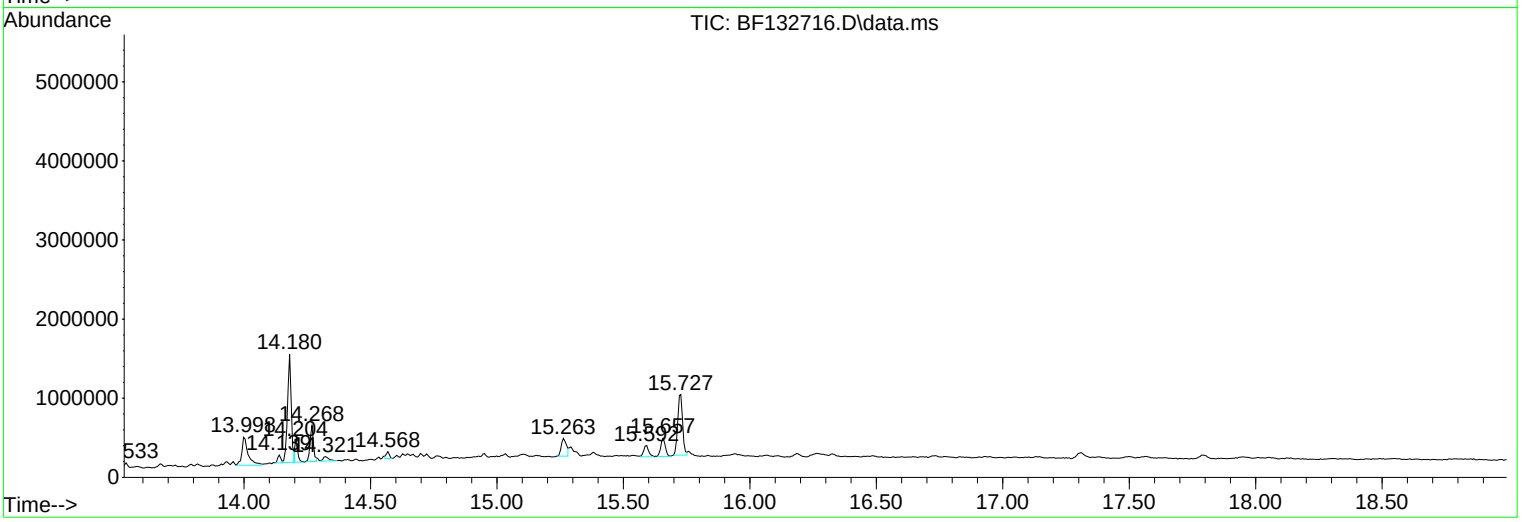
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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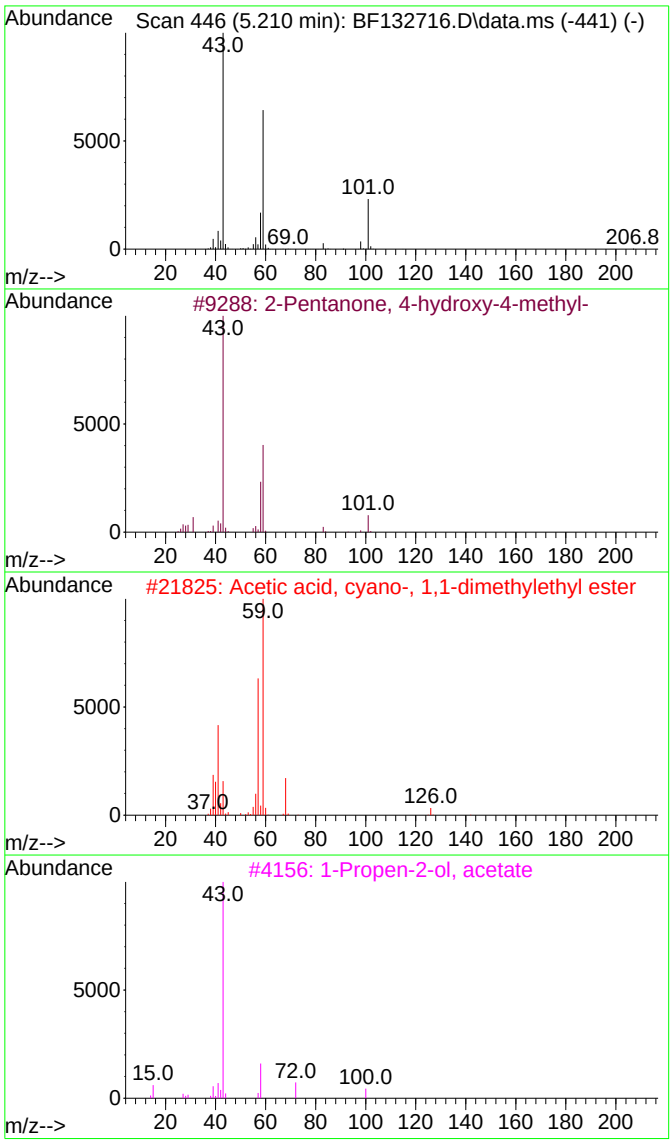
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

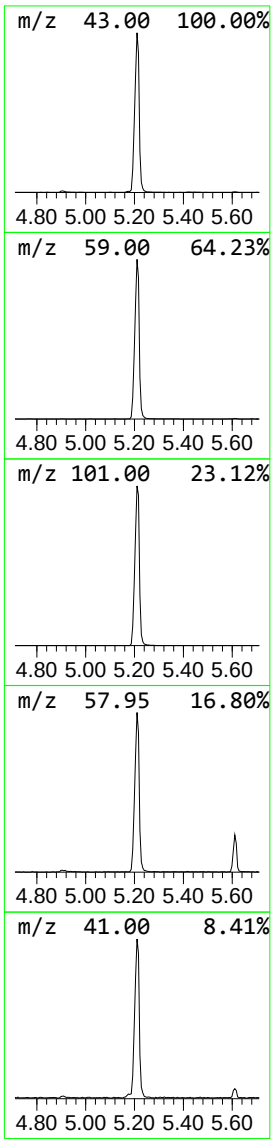
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.210	41.17 ng	2158720	1,4-Dichlorobenzene-d4	6.981

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Guanidine	59	CH5N3	000113-00-8	9





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Operator : CG\JU
Sample : 01834-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

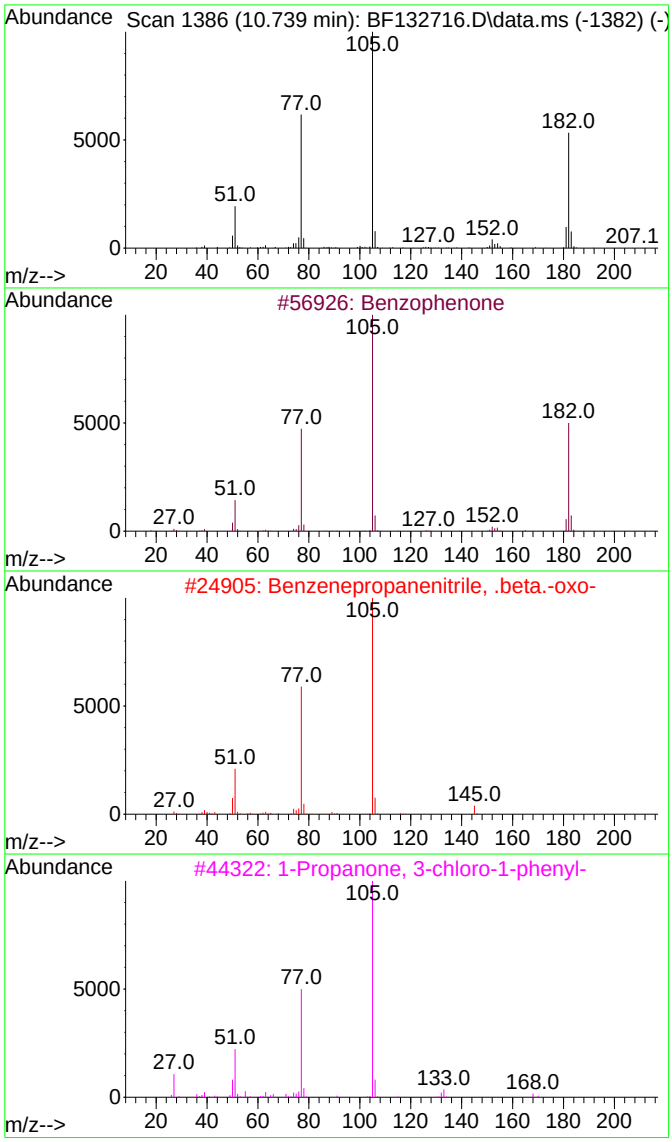
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

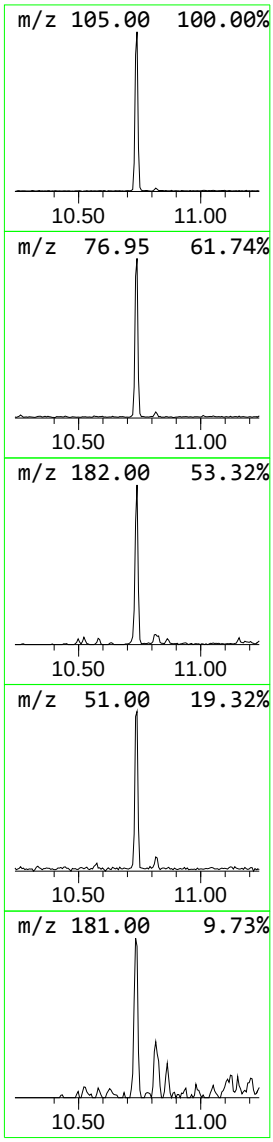
****

Peak Number 2 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.739	3.67 ng	263107	Acenaphthene-d10	10.028

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47
3	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
4	Methyl 2-benzoyl-4-cyanobutanoate	231	C13H13NO3	1010486-83-8	47
5	2-Phenylbutenolide	160	C10H8O2	001955-39-1	47





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Data File : BF132716.D
Acq On : 09 Mar 2023 14:03
Operator : CG\JU
Sample : 01834-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

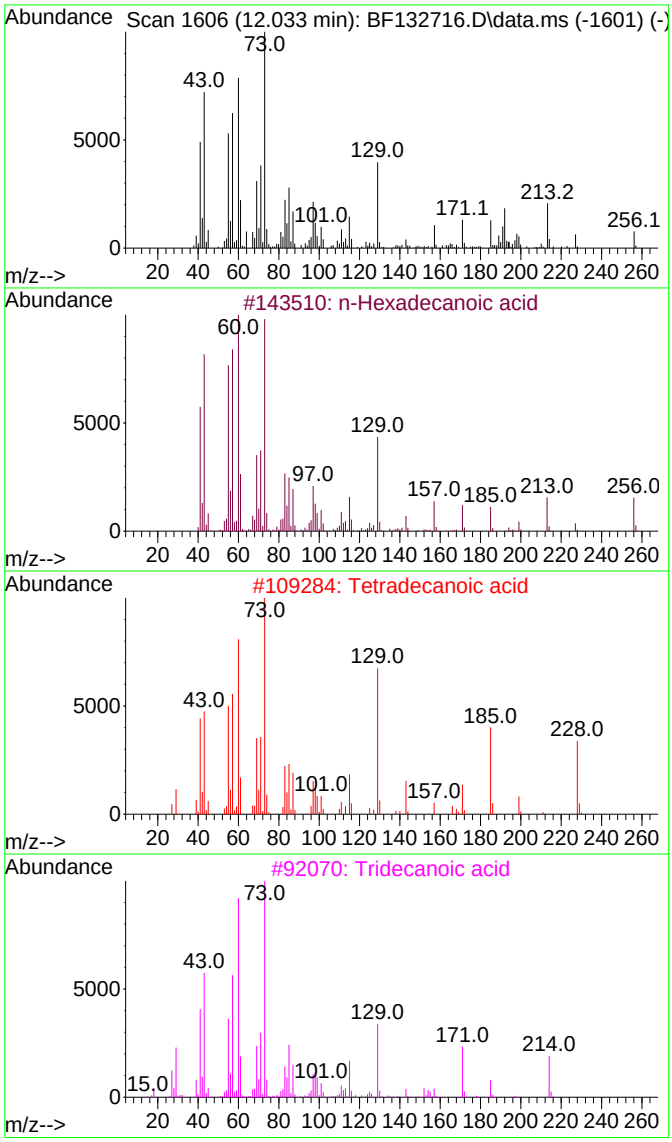
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

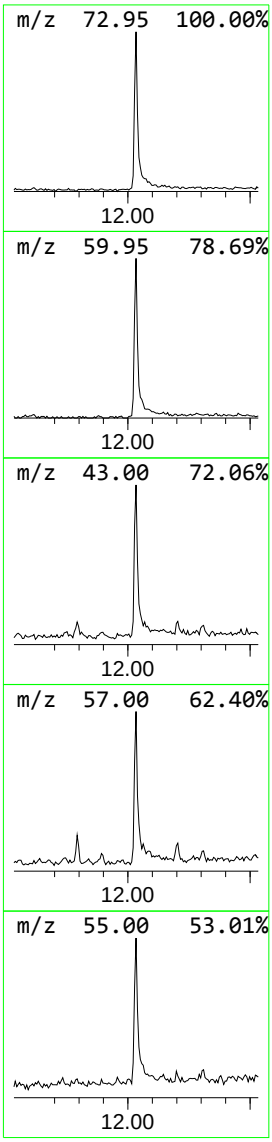
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.033	5.26 ng	335614	Phenanthrene-d10	11.522

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	87
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Dodecanoic acid	200	C12H24O2	000143-07-7	62





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Sample : 01834-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-10

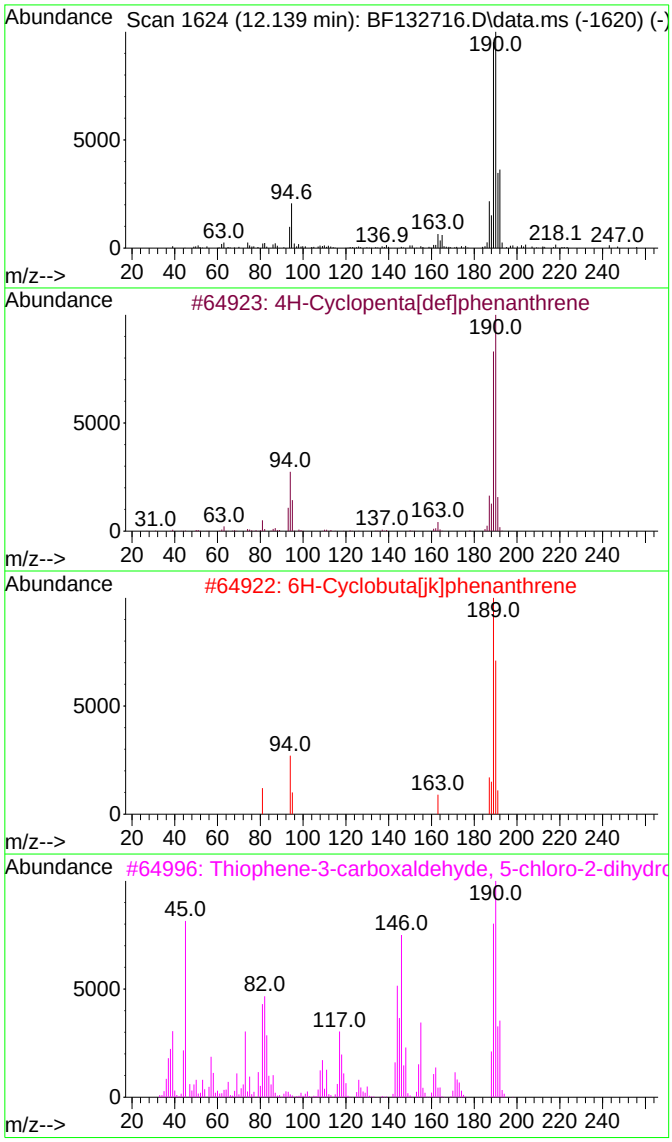
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

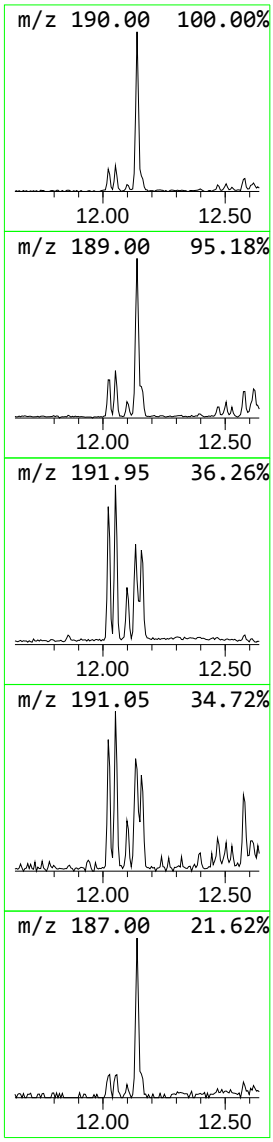
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.139	2.93 ng	186997	Phenanthrene-d10	11.522

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	72
3	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	52
4	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	50
5	Methyl diselenide	190	C2H6Se2	007101-31-7	46





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

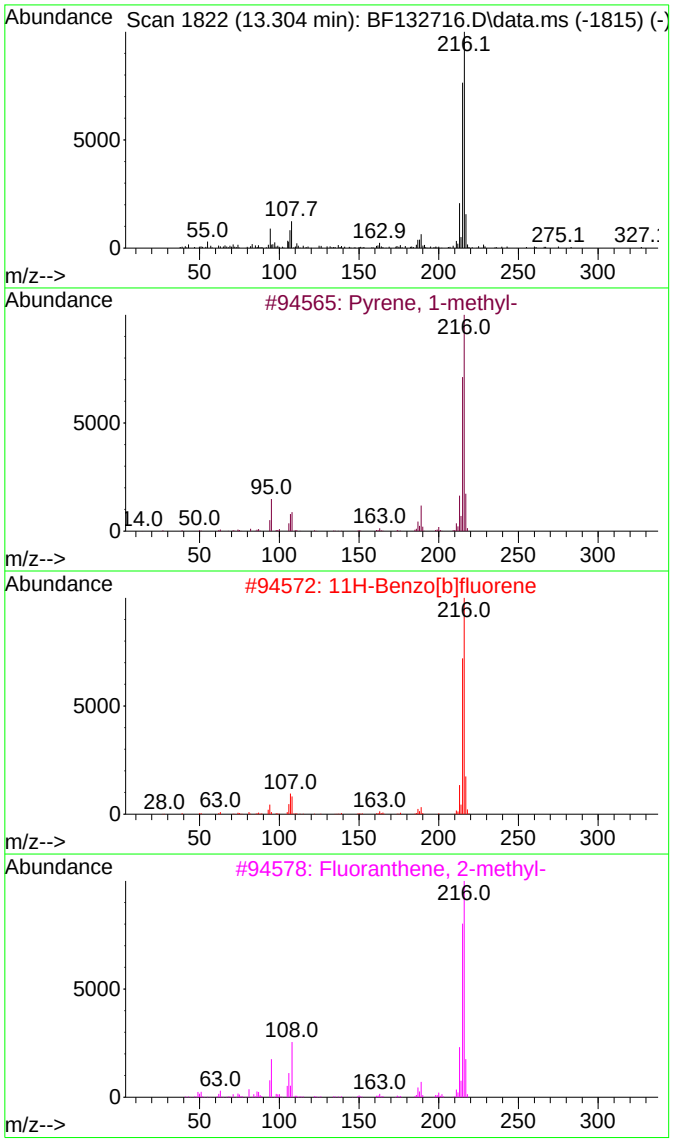
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

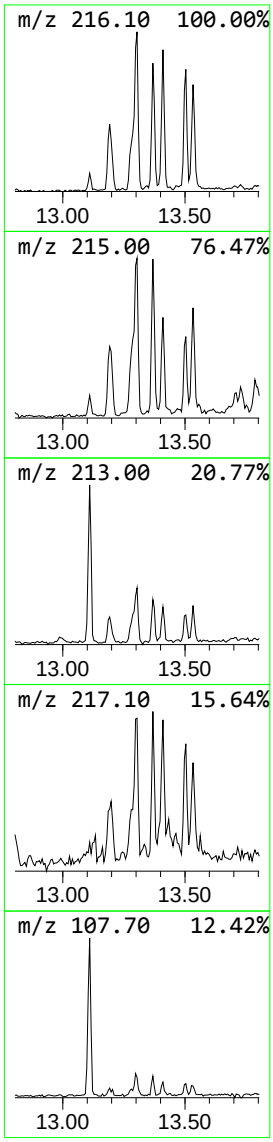
****

Peak Number 5 Pyrene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.304	2.44 ng	172630	Chrysene-d12	14.180

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	93
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	91
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	72





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Misc :
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Instrument :
BNA_F
ClientSampleId :
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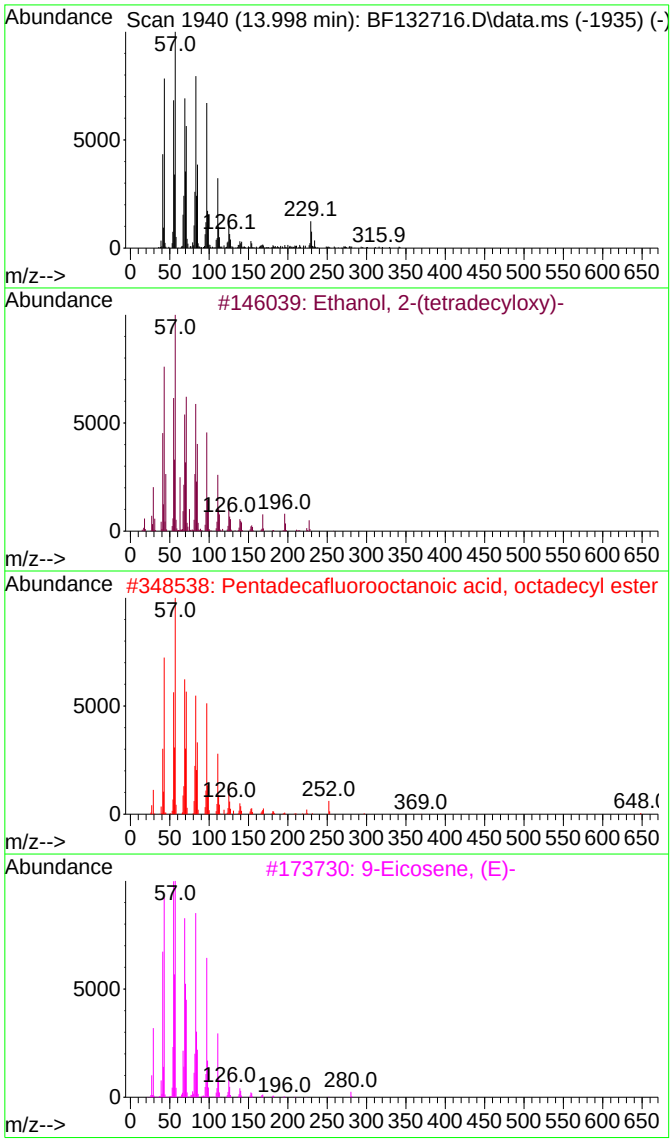
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

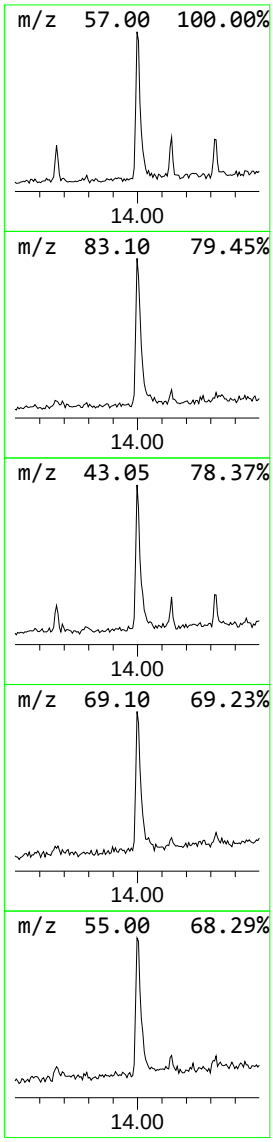
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Ethanol, 2-(tetradecyloxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.998	8.54 ng	603588	Chrysene-d12	14.180

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
2	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	89
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	89
4	1-Nonadecene	266	C19H38	018435-45-5	76
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	76





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Data File : BF132716.D
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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

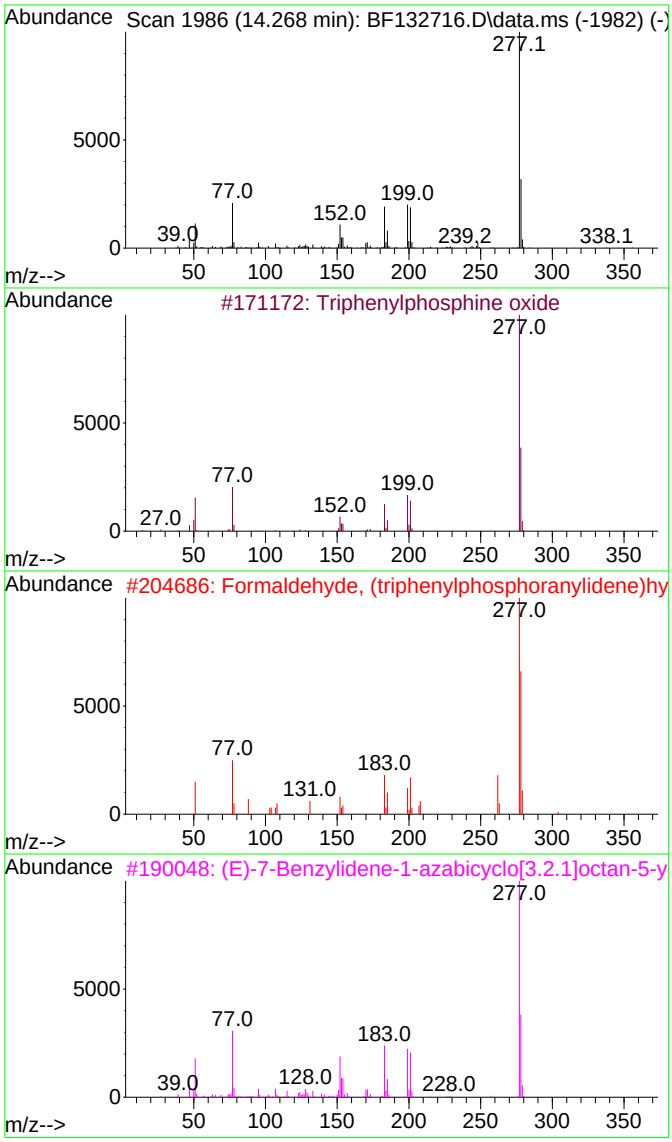
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

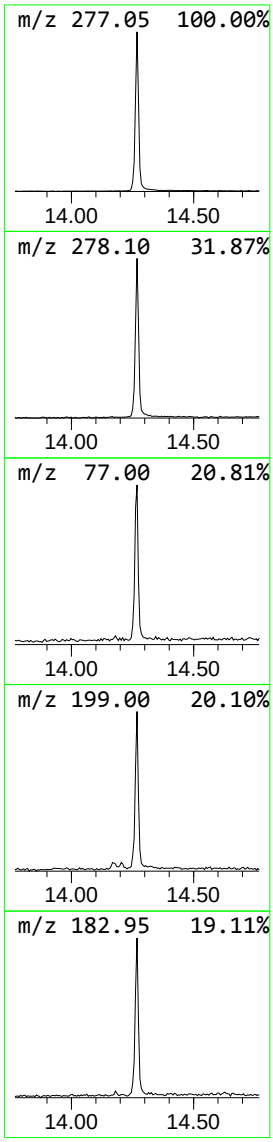
****

Peak Number 7 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.269	6.14 ng	433913	Chrysene-d12	14.180

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	94
2	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
3	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	49
4	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	40
5	2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030923\
Data File : BF132716.D
Acq On : 09 Mar 2023 14:03
Operator : CG\JU
Sample : 01834-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.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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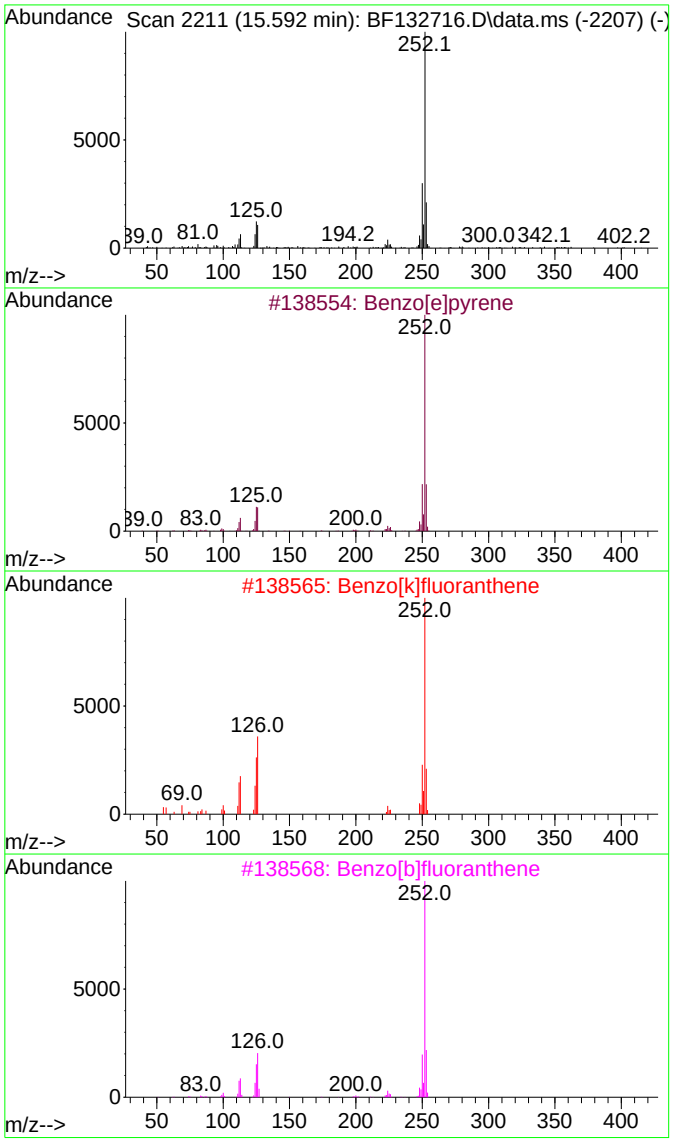
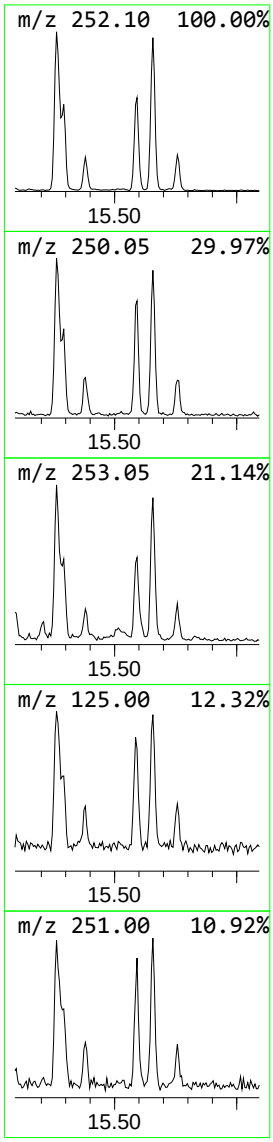
Peak Number 8 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.592	3.80 ng	196164	Perylene-d12	15.727

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
4	Benzo[a]pyrene	252	C20H12	000050-32-8	96
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	95





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030923\
Data File : BF132716.D
Acq On : 09 Mar 2023 14:03
Operator : CG\JU
Sample : 01834-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.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-...	5.210	41.2	ng	2158720	1	6.981	1048600	20.0
Benzophenone	10.739	3.7	ng	263107	3	10.028	1432810	20.0
n-Hexadecanoic ...	12.033	5.3	ng	335614	4	11.522	1276800	20.0
4H-Cyclopenta[d...	12.139	2.9	ng	186997	4	11.522	1276800	20.0
Pyrene, 1-methyl-	13.304	2.4	ng	172630	5	14.180	1413220	20.0
Ethanol, 2-(tet...	13.998	8.5	ng	603588	5	14.180	1413220	20.0
Triphenylphosph...	14.269	6.1	ng	433913	5	14.180	1413220	20.0
Benzo[e]pyrene	15.592	3.8	ng	196164	6	15.727	1031490	20.0