LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138381.D
Acq On : 27 Jun 2024 22:38
Operator : CG\JU
Sample : P3076-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 7-B-1

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-BF061224.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138381.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	7	14	20	rBV	2032798	2554427	82.24%	6.985%
2	2.281	28	33	39	rBV	30161	39595	1.27%	0.108%
3	3.399	220	223	232	rBV	41038	102027	3.28%	0.279%
4	5.099	508	512	519	rVB	234181	260386	8.38%	0.712%
5	5.510	577	582	585	rBV	3274119	3105991	100.00%	8.493%
6	6.516	748	753	756	rBV	3382374	2968591	95.58%	8.117%
7	6.704	782	785	790	rBV	53609	46342	1.49%	0.127%
8	6.881	811	815	818	rBV	1507872	1172814	37.76%	3.207%
9	7.440	906	910	913	rBV	2229783	1860962	59.92%	5.089%
10	7.692	950	953	959	rVB	114348	87092	2.80%	0.238%
11	8.157	1029	1032	1035	rBV	1550958	1330624	42.84%	3.639%
12	8.469	1081	1085	1094	rBV	169353	150085	4.83%	0.410%
13	9.234	1211	1215	1218	rBV	3612643	2847158	91.67%	7.785%
14	9.910	1327	1330	1333	rBV	1448218	1139060	36.67%	3.115%
15	9.945	1333	1336	1339	rVB	121421	101737	3.28%	0.278%
16	10.010	1343	1347	1352	rVB2	70682	94783	3.05%	0.259%
17	10.116	1361	1365	1369	rVB2	51516	46244	1.49%	0.126%
18	10.457	1420	1423	1428	rVB	115438	96676	3.11%	0.264%
19	10.698	1460	1464	1468	rBV	1972536	1597820	51.44%	4.369%
20	11.004	1510	1516	1519	rBV3	34292	42481	1.37%	0.116%
21	11.257	1553	1559	1561	rBV2	24103	38122	1.23%	0.104%
22	11.292	1562	1565	1571	rVB	63245	60027	1.93%	0.164%
23	11.398	1579	1583	1585	rBV	1356189	1166422	37.55%	3.190%
24	11.422	1585	1587	1590	rVV	1279925	923543	29.73%	2.525%
25	11.469	1592	1595	1599	rVB	289212	267203	8.60%	0.731%
26	11.628	1619	1622	1630	rVB	47909	48339	1.56%	0.132%
27	11.898	1662	1668	1670	rBV	123750	117001	3.77%	0.320%
28	11.922	1670	1672	1677	rVV2	302724	306621	9.87%	0.838%
29	11.975	1678	1681	1683	rVV	80001	81431	2.62%	0.223%
30	12.010	1683	1687	1689	rVV	235040	234593	7.55%	0.641%
31	12.033	1689	1691	1695	rVB	82057	67544	2.17%	0.185%
32	12.192	1715	1718	1720	rBV	97549	76646	2.47%	0.210%
33	12.216	1720	1722	1725	rVB2	48066	38239	1.23%	0.105%
34	12.445	1758	1761	1764	rBV	66140	71639	2.31%	0.196%
35	12.486	1764	1768	1770	rVV2	51125	59242	1.91%	0.162%
36	12.533	1773	1776	1781	rBV3	50344	61629	1.98%	0.169%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138381.D
Acq On : 27 Jun 2024 22:38
Operator : CG\JU
Sample : P3076-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
7-B-1

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-BF061224.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.610	1785	1789	1792	rBV	1922664	1566062	50.42%	4.282%
38	12.704	1802	1805	1807	rBV2	62377	55895	1.80%	0.153%
39	12.763	1812	1815	1818	rVB	48814	44015	1.42%	0.120%
40	12.839	1822	1828	1833	rVB	1565665	1557475	50.14%	4.259%
41	12.886	1833	1836	1841	rVB2	62381	75177	2.42%	0.206%
42	12.957	1845	1848	1849	rBV	76507	70170	2.26%	0.192%
43	12.980	1849	1852	1855	rVV	3624725	2993865	96.39%	8.187%
44	13.057	1860	1865	1868	rBV2	73968	129691	4.18%	0.355%
45	13.139	1876	1879	1881	rBV3	56124	71570	2.30%	0.196%
46	13.163	1881	1883	1886	rVB	204945	182664	5.88%	0.499%
47	13.210	1886	1891	1892	rBV4	32629	39368	1.27%	0.108%
48	13.233	1892	1895	1897	rVB	178669	143866	4.63%	0.393%
49	13.269	1897	1901	1904	rBV2	126144	118296	3.81%	0.323%
50	13.363	1914	1917	1919	rBV	63254	47944	1.54%	0.131%
51	13.392	1919	1922	1925	rBV2	58579	58792	1.89%	0.161%
52	13.669	1967	1969	1974	rVB	56313	56455	1.82%	0.154%
53	13.786	1985	1989	1991	rBV3	85654	101016	3.25%	0.276%
54	13.810	1991	1993	1995	rVV	99211	88149	2.84%	0.241%
55	13.833	1995	1997	2001	rVV2	91784	123630	3.98%	0.338%
56	13.874	2001	2004	2014	rVB2	256083	313899	10.11%	0.858%
57	14.033	2023	2031	2034	rBV2	1583462	2062116	66.39%	5.639%
58	14.057	2034	2035	2041	rVB	566502	486374	15.66%	1.330%
59	14.139	2046	2049	2052	rVB	163712	129709	4.18%	0.355%
60	14.421	2094	2097	2100	rVB	77201	68916	2.22%	0.188%
61	14.451	2100	2102	2106	rVB	40218	36146	1.16%	0.099%
62	14.504	2108	2111	2115	rBV3	67074	112758	3.63%	0.308%
63	15.074	2204	2208	2211	rBV	383160	553090	17.81%	1.512%
64	15.151	2218	2221	2224	rBV	50517	57634	1.86%	0.158%
65	15.180	2224	2226	2230	rVB	74623	79374	2.56%	0.217%
66	15.380	2256	2260	2266	rVB	186004	241853	7.79%	0.661%
67	15.439	2266	2270	2276	rVB	304618	364787	11.74%	0.997%
68	15.504	2277	2281	2285	rBV	730163	878643	28.29%	2.403%
69	16.968	2526	2530	2540	rVB2	112919	220853	7.11%	0.604%
70	17.415	2602	2606	2617	rVB	90458	177073	5.70%	0.484%

Sum of corrected areas: 36570461

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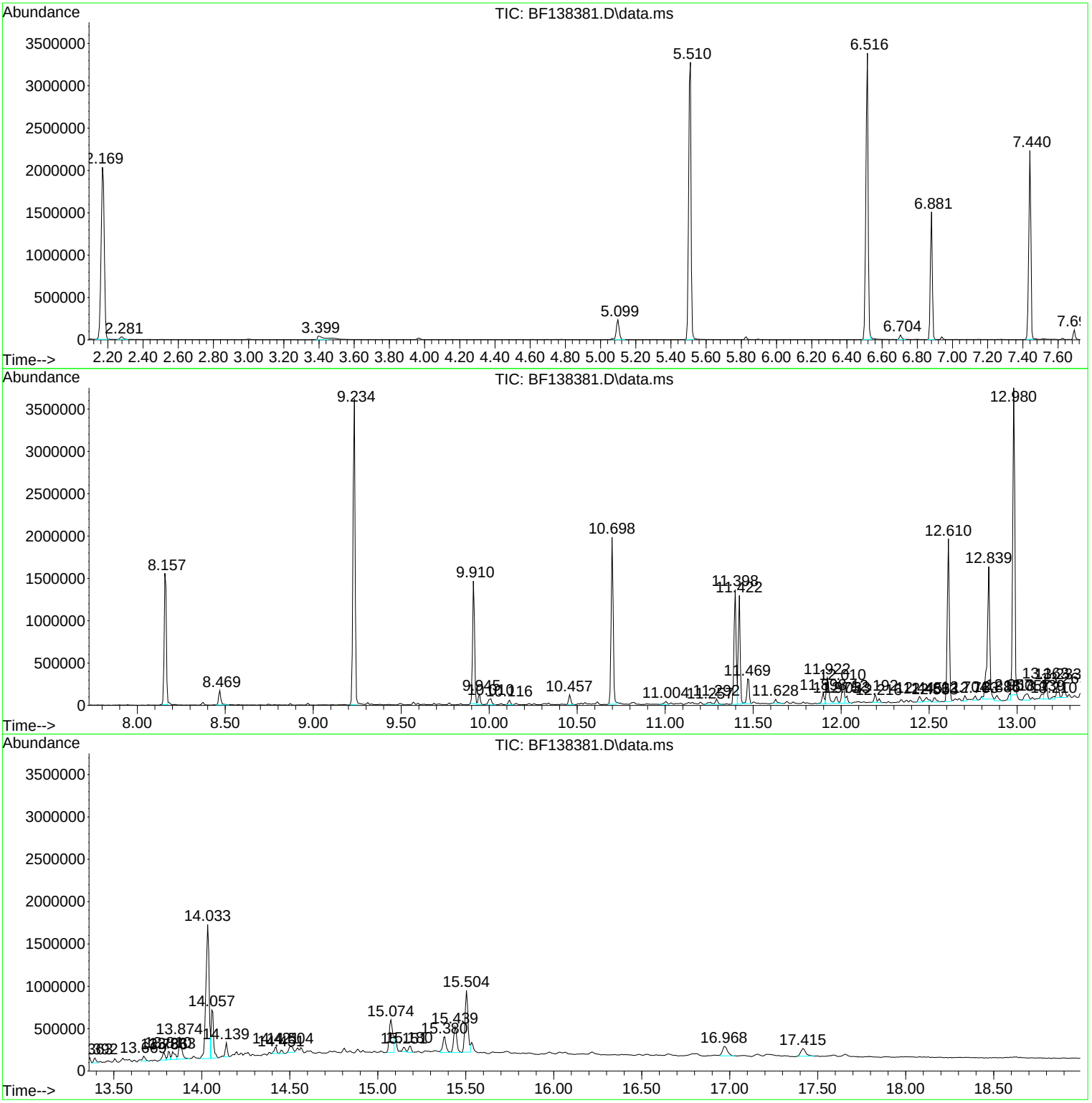
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
7-B-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
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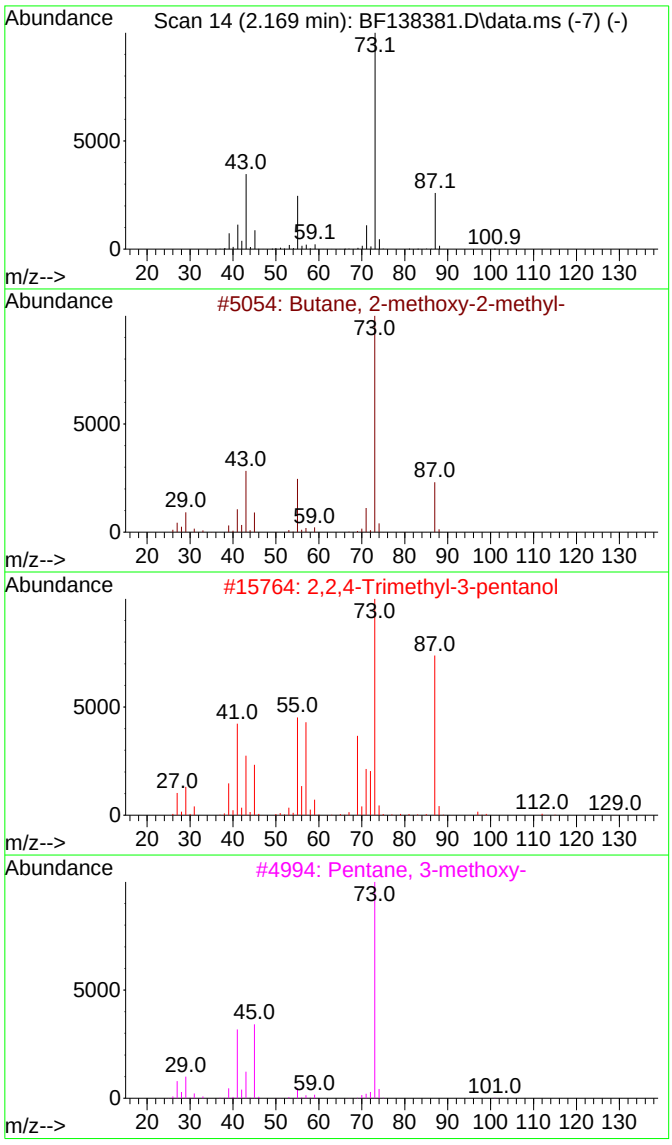
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

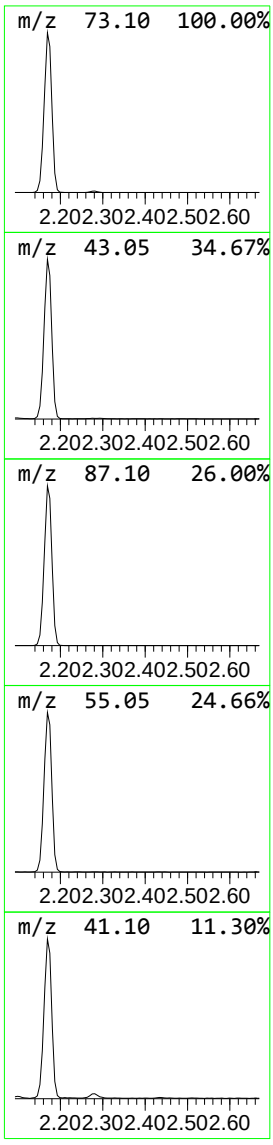
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	43.56 ng	2554430	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





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Data File : BF138381.D
Acq On : 27 Jun 2024 22:38
Operator : CG\JU
Sample : P3076-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
7-B-1

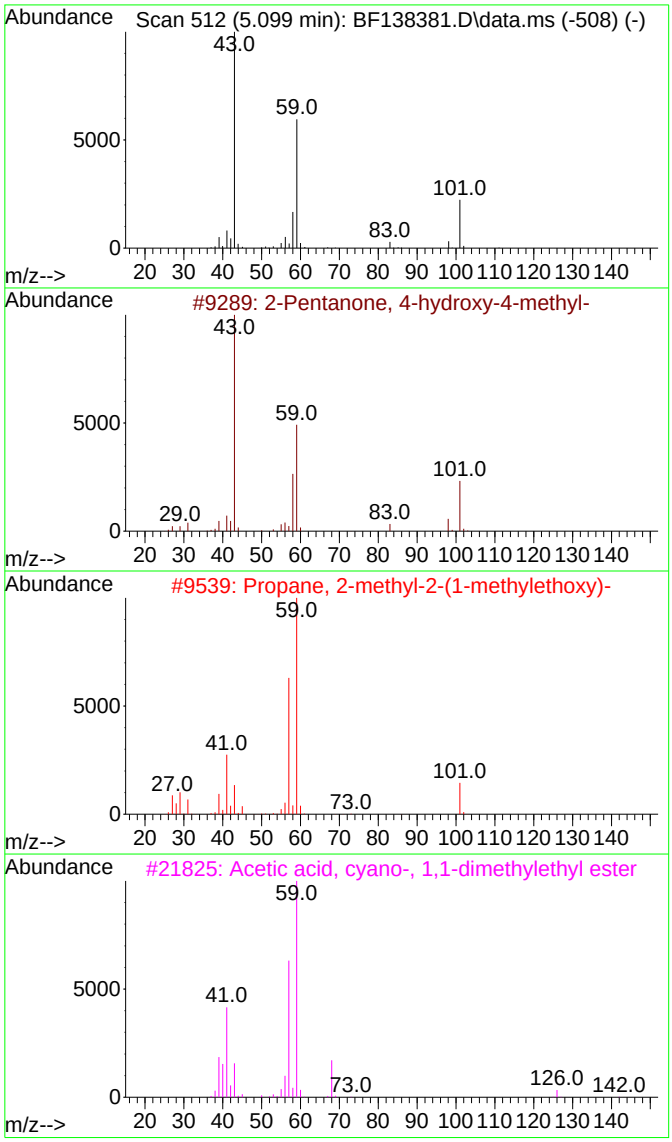
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

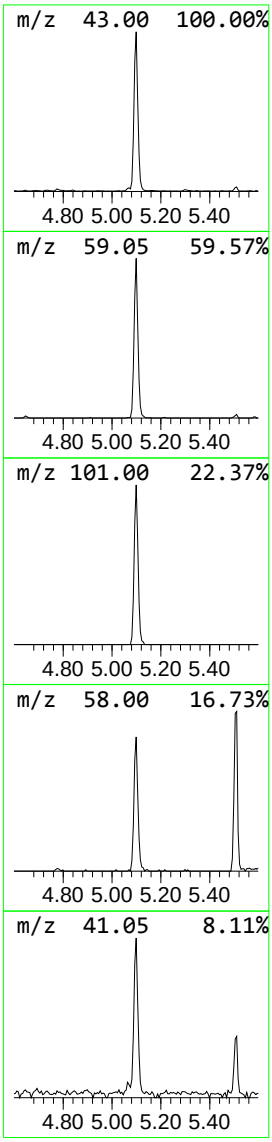
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.099	4.44 ng	260386	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Guanidine	59	CH5N3	000113-00-8	9





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

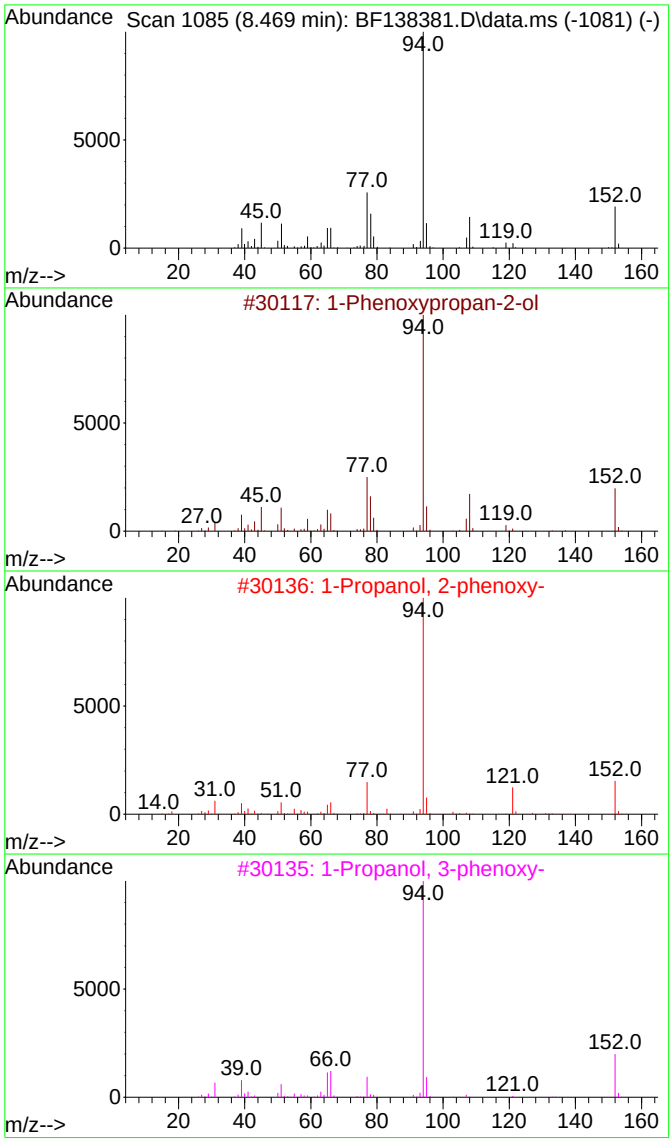
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

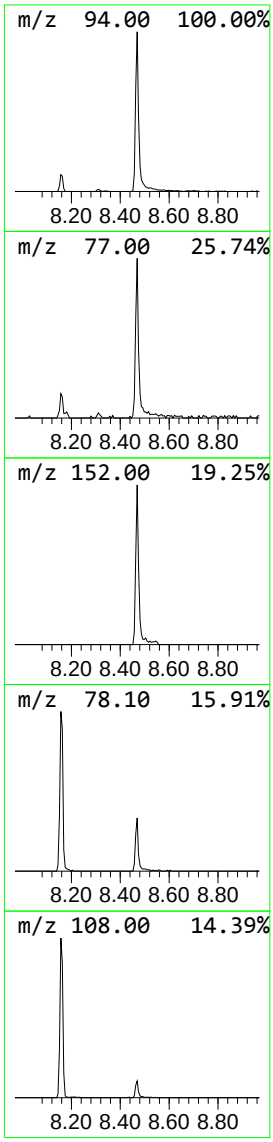
****

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.469	2.26 ng	150085	Naphthalene-d8	8.157

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	72
3	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	64
4	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	59
5	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	53





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

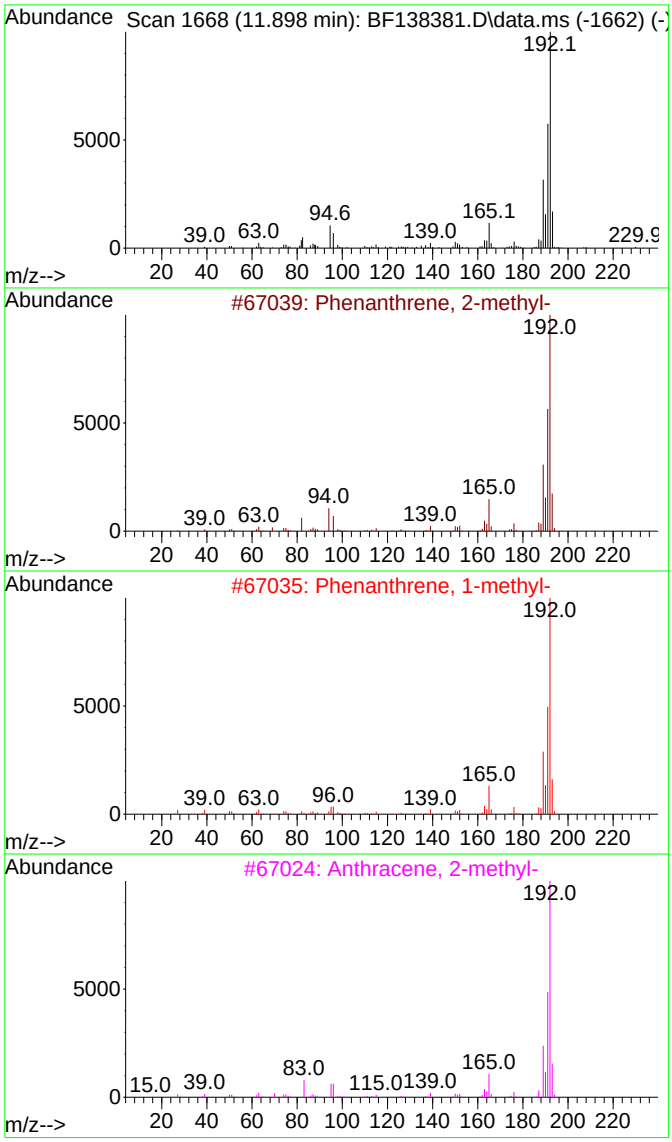
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

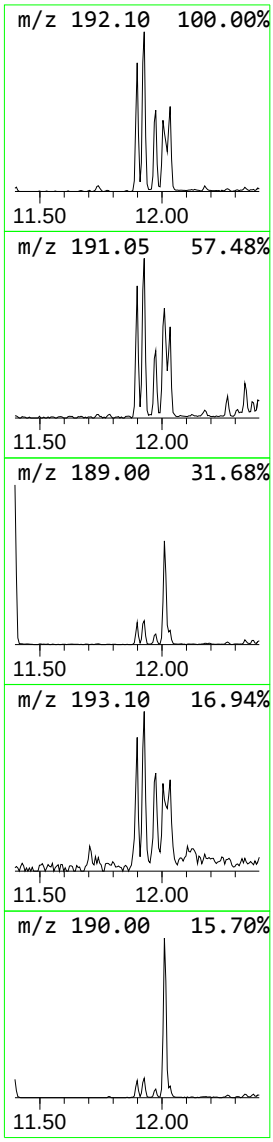
****

Peak Number 4 Phenanthrene, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	2.01 ng	117001	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	91
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	90





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Operator : CG\JU
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

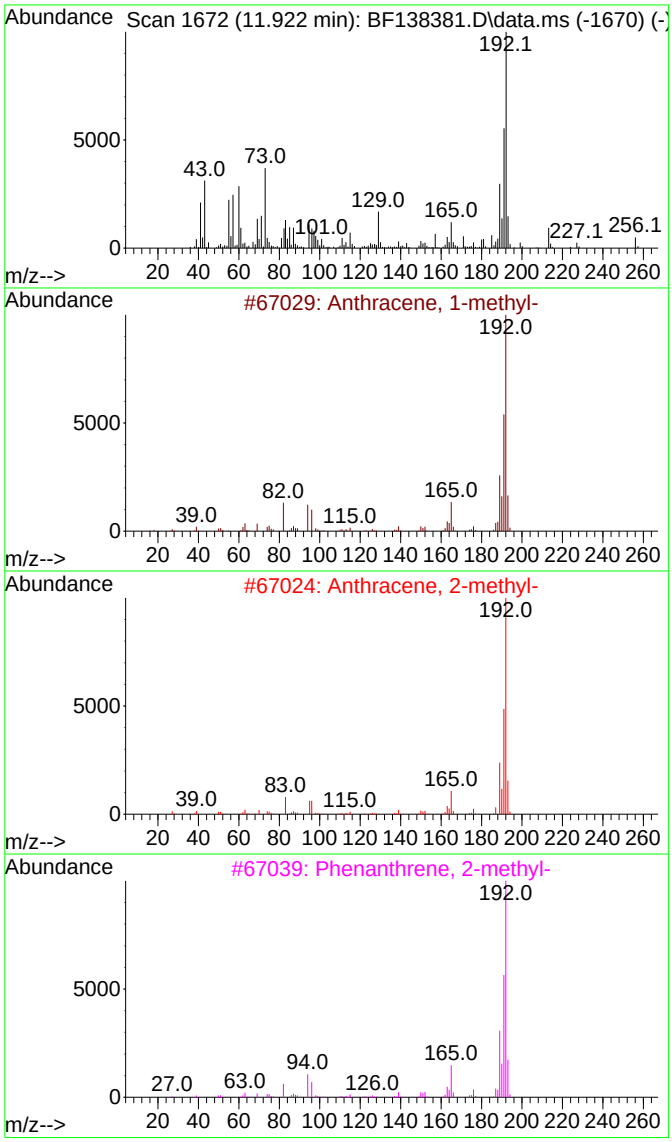
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

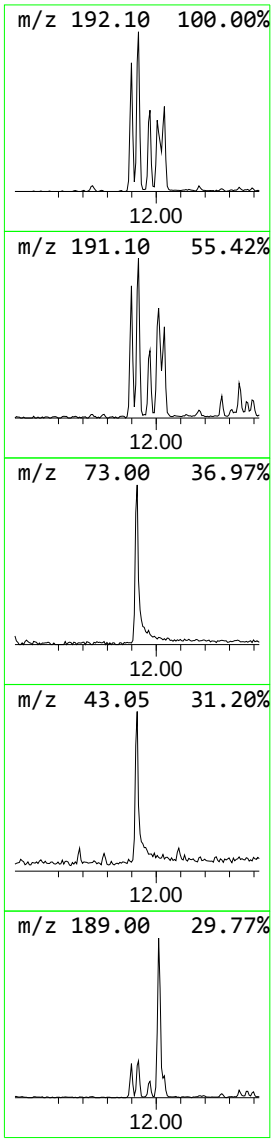
****

Peak Number 5 Anthracene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	5.26 ng	306621	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	97
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	97
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	97
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	93





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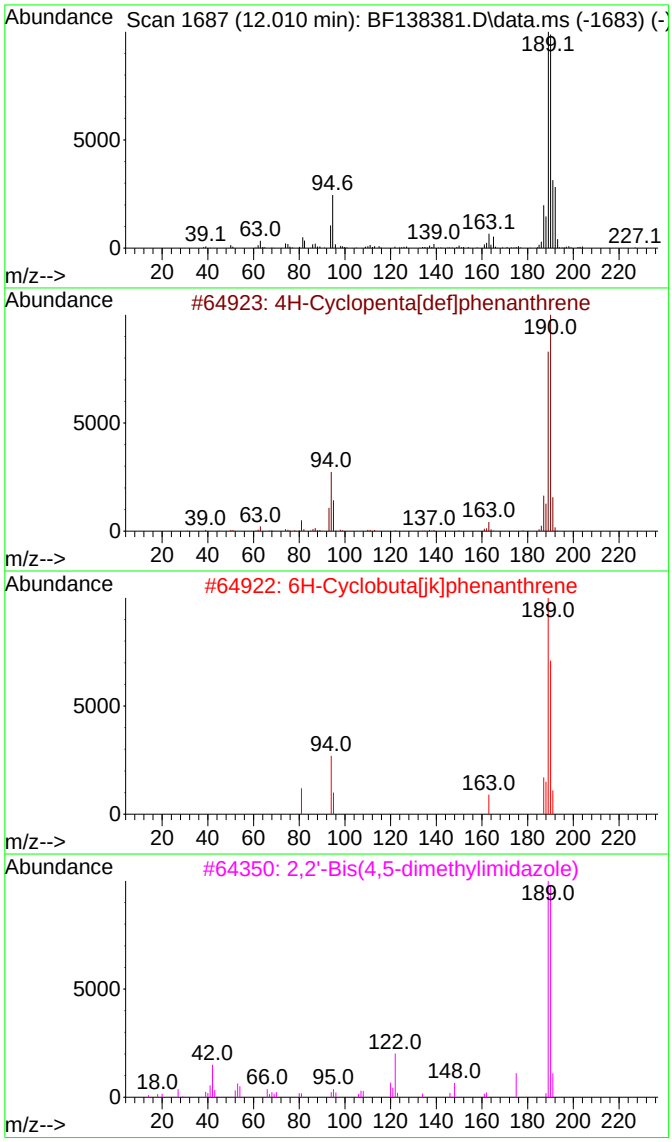
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

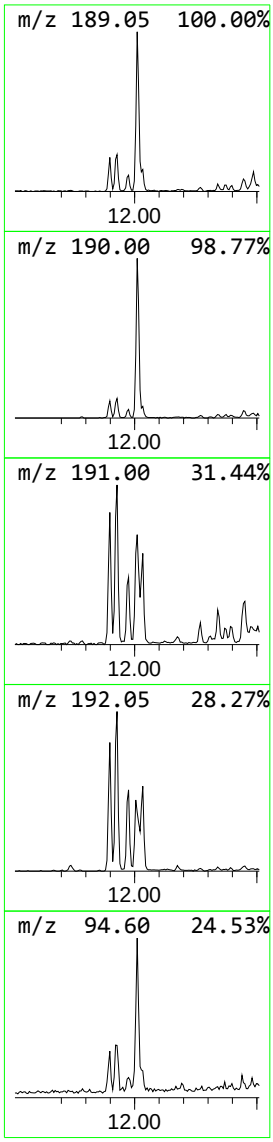
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.010	4.02 ng	234593	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	94
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	64
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40
4	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	17
5	1-(Phenylethynyl)-1H-1,2,3-benzo...	219	C14H9N3	209912-23-2	16





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138381.D
Acq On : 27 Jun 2024 22:38
Operator : CG\JU
Sample : P3076-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
7-B-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

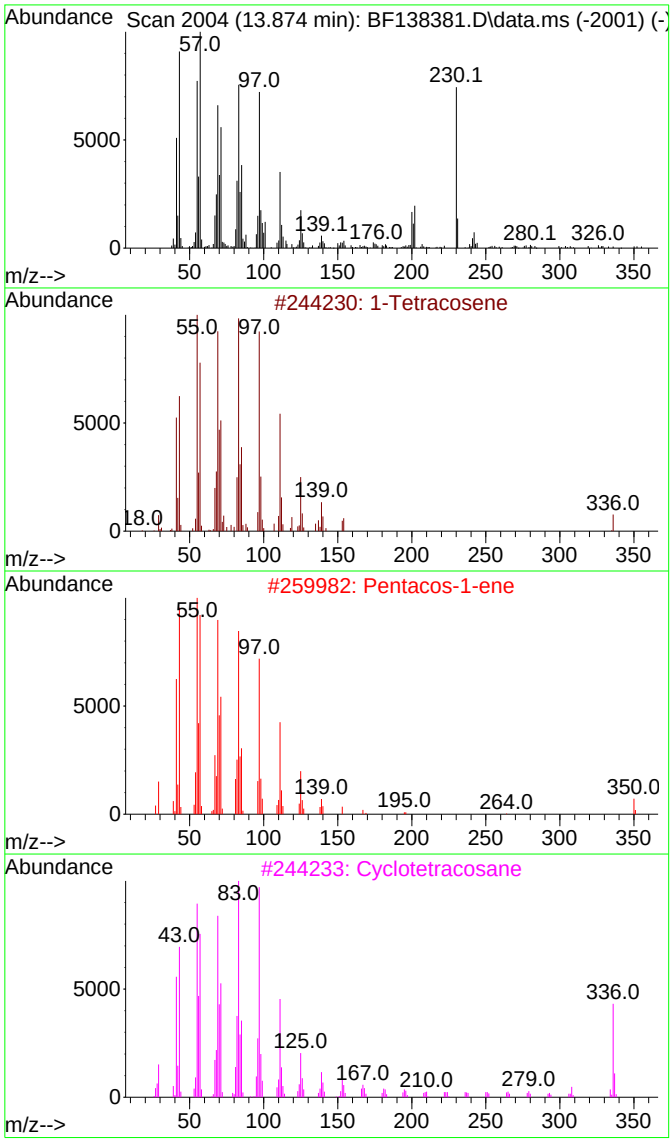
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

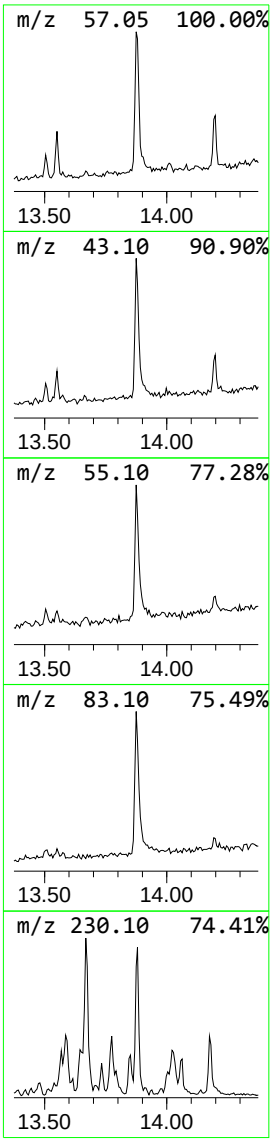
****

Peak Number 7 1-Tetracosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	3.04 ng	313899	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene	336	C24H48	010192-32-2	96
2	Pentacos-1-ene	350	C25H50	016980-85-1	91
3	Cyclotetracosane	336	C24H48	000297-03-0	90
4	1-Heneicosanol	312	C21H44O	015594-90-8	86
5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138381.D
Acq On : 27 Jun 2024 22:38
Operator : CG\JU
Sample : P3076-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
7-B-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

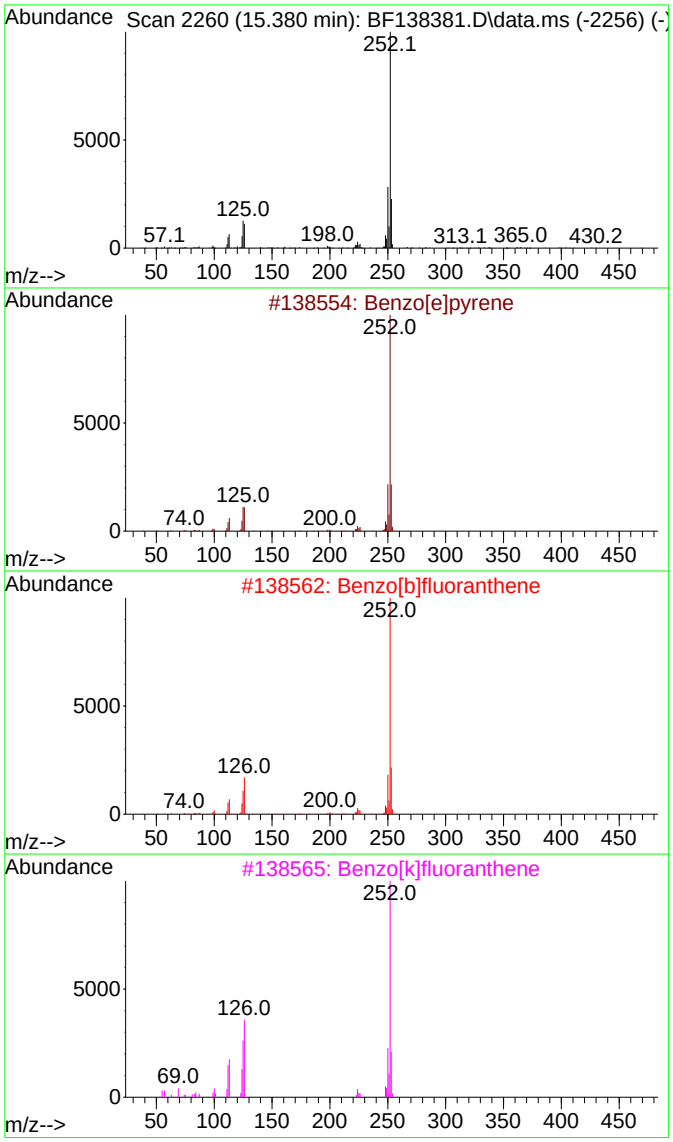
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

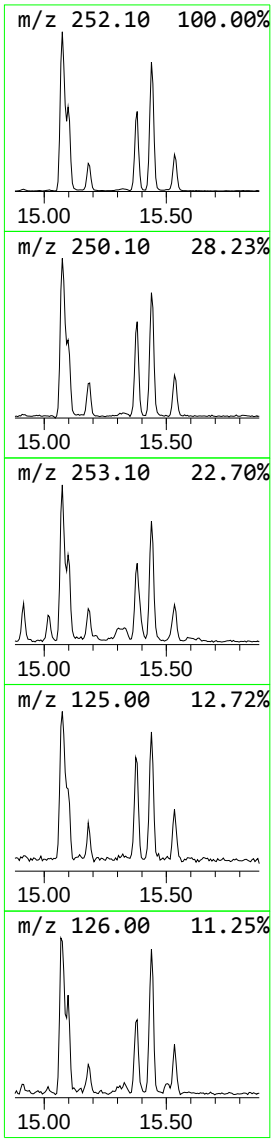
****

Peak Number 8 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.380	5.51 ng	241853	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
4	Benzo[a]pyrene	252	C20H12	000050-32-8	95
5	Perylene	252	C20H12	000198-55-0	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138381.D
Acq On : 27 Jun 2024 22:38
Operator : CG\JU
Sample : P3076-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
7-B-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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
Butane, 2-metho...	2.169	43.6	ng	2554430	1	6.881	1172810	20.0
2-Pentanone, 4-...	5.099	4.4	ng	260386	1	6.881	1172810	20.0
1-Phenoxypropan...	8.469	2.3	ng	150085	2	8.157	1330620	20.0
Phenanthrene, 2...	11.898	2.0	ng	117001	4	11.398	1166420	20.0
Anthracene, 1-m...	11.922	5.3	ng	306621	4	11.398	1166420	20.0
4H-Cyclopenta[d...	12.010	4.0	ng	234593	4	11.398	1166420	20.0
1-Tetracosene	13.874	3.0	ng	313899	5	14.033	2062120	20.0
Benzo[e]pyrene	15.380	5.5	ng	241853	6	15.504	878643	20.0