LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133274.D
Acq On : 05 May 2023 20:50
Operator : CG\JU
Sample : 02616-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133274.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.710	271	276	282	rVB	33890	51279	1.46%	0.149%
2	4.916	476	481	490	rVB	572344	676587	19.28%	1.966%
3	5.340	549	553	556	rBV	3747595	3419285	97.43%	9.934%
4	6.369	723	728	731	rBV	3732877	3509345	100.00%	10.196%
5	6.551	755	759	765	rBV3	30245	44733	1.27%	0.130%
6	6.722	785	788	792	rBV	1277781	1100327	31.35%	3.197%
7	7.287	880	884	887	rBV	2383122	2235280	63.70%	6.494%
8	8.010	1003	1007	1009	rBV	1900461	1500607	42.76%	4.360%
9	8.028	1009	1010	1013	rVB	117715	66595	1.90%	0.193%
10	9.081	1186	1189	1192	rBV	3389786	2905355	82.79%	8.441%
11	9.616	1277	1280	1286	rVB	52560	55514	1.58%	0.161%
12	9.757	1301	1304	1308	rVB	1970934	1628285	46.40%	4.731%
13	10.304	1394	1397	1403	rVB3	31053	41292	1.18%	0.120%
14	10.469	1422	1425	1429	rVB	619522	556370	15.85%	1.616%
15	10.545	1434	1438	1442	rBV	2598991	2375948	67.70%	6.903%
16	10.669	1457	1459	1464	rVB3	45773	53471	1.52%	0.155%
17	10.851	1484	1490	1492	rBV4	33818	47617	1.36%	0.138%
18	11.239	1552	1556	1558	rBV	2017623	1663052	47.39%	4.832%
19	11.263	1558	1560	1563	rVV	363472	258723	7.37%	0.752%
20	11.310	1563	1568	1572	rVV	55893	60358	1.72%	0.175%
21	11.569	1610	1612	1618	rVB	58838	54622	1.56%	0.159%
22	11.651	1623	1626	1630	rVB	43680	46411	1.32%	0.135%
23	11.739	1638	1641	1643	rBV	175951	148005	4.22%	0.430%
24	11.775	1643	1647	1651	rVV2	374945	504466	14.37%	1.466%
25	11.816	1651	1654	1656	rVV2	72224	90492	2.58%	0.263%
26	11.851	1656	1660	1662	rVV	215479	239506	6.82%	0.696%
27	11.875	1662	1664	1669	rVB	151751	126709	3.61%	0.368%
28	12.033	1689	1691	1693	rBV	95350	81342	2.32%	0.236%
29	12.186	1715	1717	1719	rVB	53278	37660	1.07%	0.109%
30	12.216	1719	1722	1724	rBV	96486	73759	2.10%	0.214%
31	12.239	1724	1726	1728	rVB	74112	56589	1.61%	0.164%
32	12.292	1731	1735	1737	rBV	203985	203966	5.81%	0.593%
33	12.327	1737	1741	1743	rVV	110618	150454	4.29%	0.437%
34	12.345	1743	1744	1746	rVB	79373	42315	1.21%	0.123%
35	12.375	1746	1749	1753	rBV2	82705	111404	3.17%	0.324%
36	12.445	1758	1761	1767	rBV	397175	408445	11.64%	1.187%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133274.D
Acq On : 05 May 2023 20:50
Operator : CG\JU
Sample : 02616-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.675	1795	1800	1803	rBV	730145	664298	18.93%	1.930%
38	12.704	1803	1805	1808	rVV3	72662	85201	2.43%	0.248%
39	12.739	1808	1811	1814	rVB2	90773	97126	2.77%	0.282%
40	12.827	1822	1826	1829	rBV	2704818	2547677	72.60%	7.402%
41	12.898	1834	1838	1845	rVB3	109558	157952	4.50%	0.459%
42	12.986	1849	1853	1854	rBV3	76356	92312	2.63%	0.268%
43	13.004	1854	1856	1859	rVB	134208	117756	3.36%	0.342%
44	13.069	1861	1867	1871	rBV3	100544	135213	3.85%	0.393%
45	13.110	1871	1874	1877	rBV	174076	152797	4.35%	0.444%
46	13.198	1886	1889	1892	rVB	135927	120408	3.43%	0.350%
47	13.233	1892	1895	1898	rVB	124498	111398	3.17%	0.324%
48	13.410	1922	1925	1927	rBV2	52307	49850	1.42%	0.145%
49	13.510	1940	1942	1947	rVB	64184	81998	2.34%	0.238%
50	13.622	1957	1961	1964	rBV3	61498	90282	2.57%	0.262%
51	13.733	1976	1980	1988	rBV3	238834	366083	10.43%	1.064%
52	13.874	1998	2004	2006	rBV2	1420898	1519136	43.29%	4.414%
53	13.898	2006	2008	2013	rVB	266613	229654	6.54%	0.667%
54	13.969	2015	2020	2025	rBV	940461	944884	26.92%	2.745%
55	14.051	2032	2034	2042	rVB3	66178	63992	1.82%	0.186%
56	14.257	2065	2069	2073	rBV	106903	122238	3.48%	0.355%
57	14.292	2073	2075	2078	rVB	74277	57048	1.63%	0.166%
58	14.357	2083	2086	2088	rBV2	75034	69939	1.99%	0.203%
59	14.386	2088	2091	2092	rBV	42865	37070	1.06%	0.108%
60	14.886	2172	2176	2183	rBV	129955	231992	6.61%	0.674%
61	14.974	2188	2191	2195	rBV2	46422	66964	1.91%	0.195%
62	15.168	2220	2224	2229	rVB	112414	125385	3.57%	0.364%
63	15.227	2230	2234	2239	rBV	141736	166097	4.73%	0.483%
64	15.292	2240	2245	2248	rBV	910908	1030154	29.35%	2.993%
65	15.739	2318	2321	2325	rBV	40068	52710	1.50%	0.153%
66	16.657	2473	2477	2483	rVB3	59022	104809	2.99%	0.305%
67	17.068	2542	2547	2553	rVB2	54988	100872	2.87%	0.293%

Sum of corrected areas: 34419463

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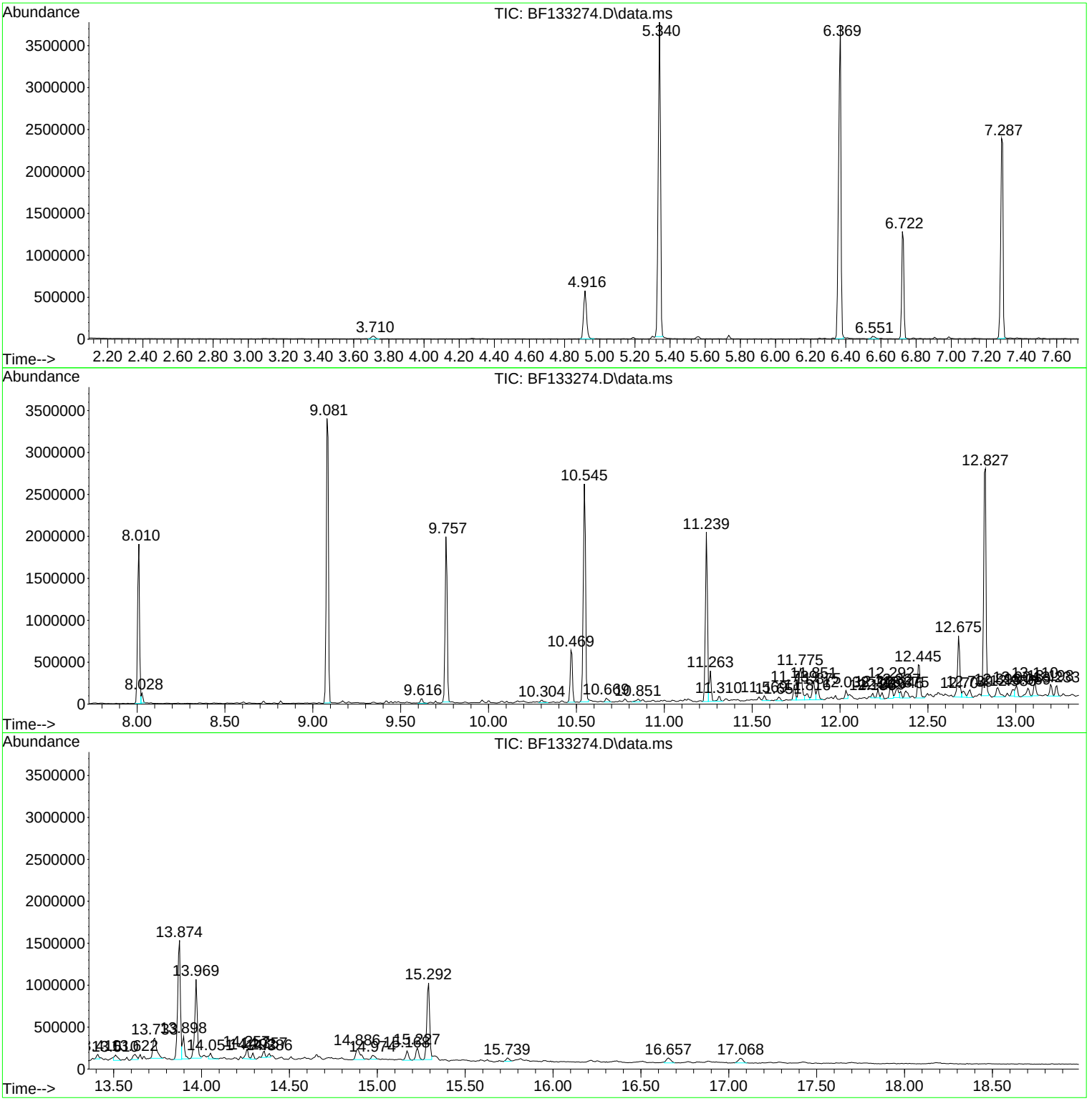
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133274.D
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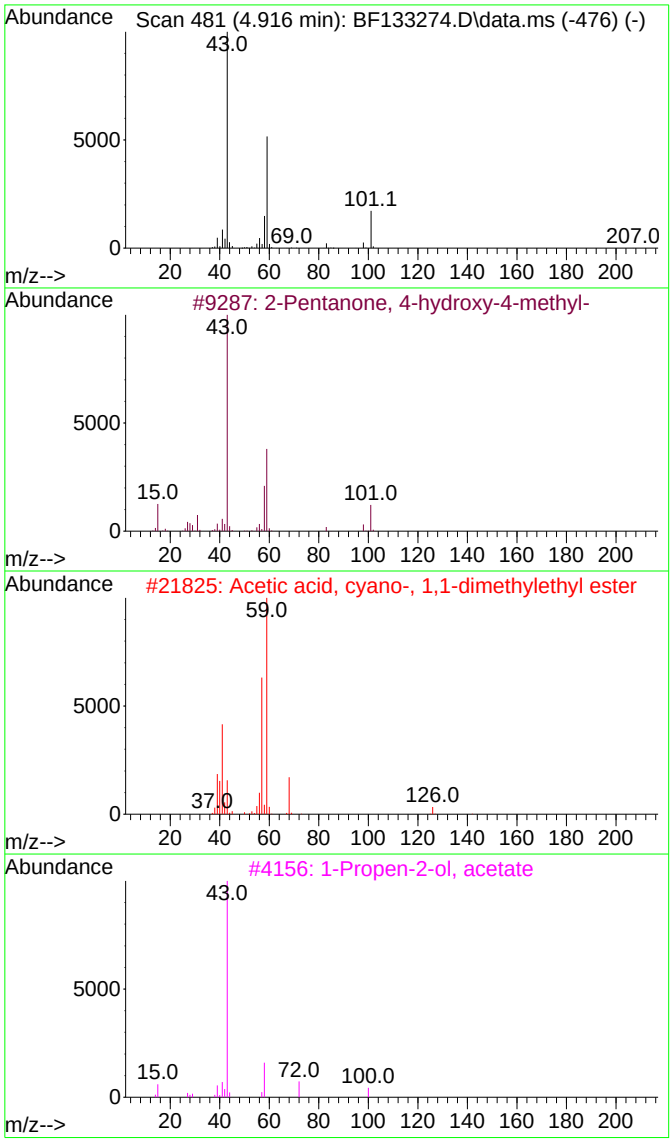
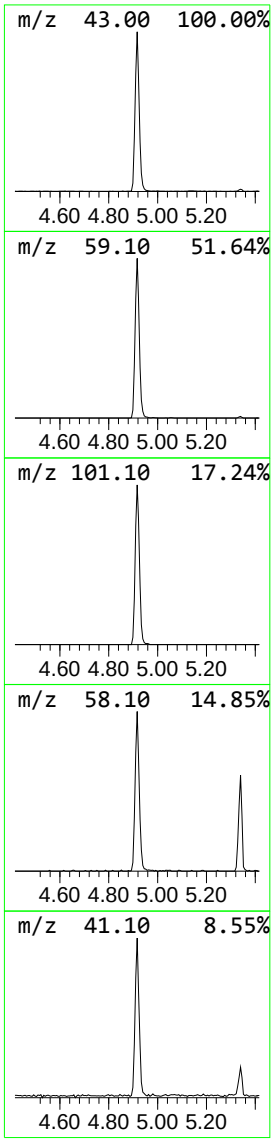
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.916	12.30 ng	676587	1,4-Dichlorobenzene-d4	6.728

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	3-Hexanol	102	C6H14O	000623-37-0	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133274.D
Acq On : 05 May 2023 20:50
Operator : CG\JU
Sample : 02616-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

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

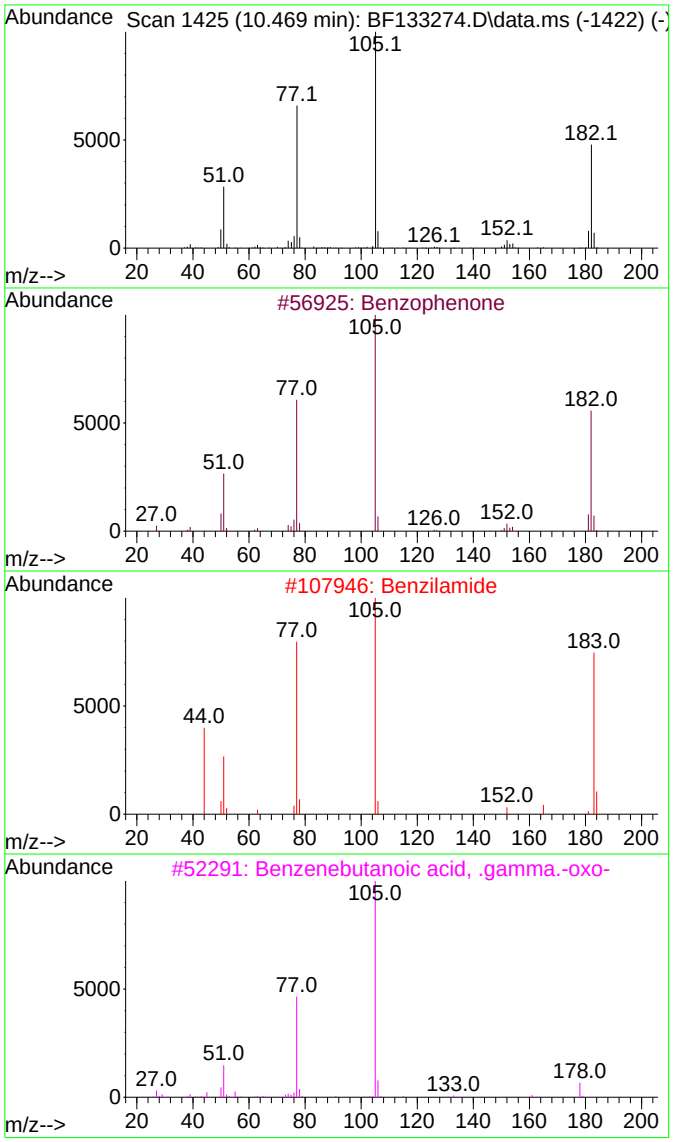
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

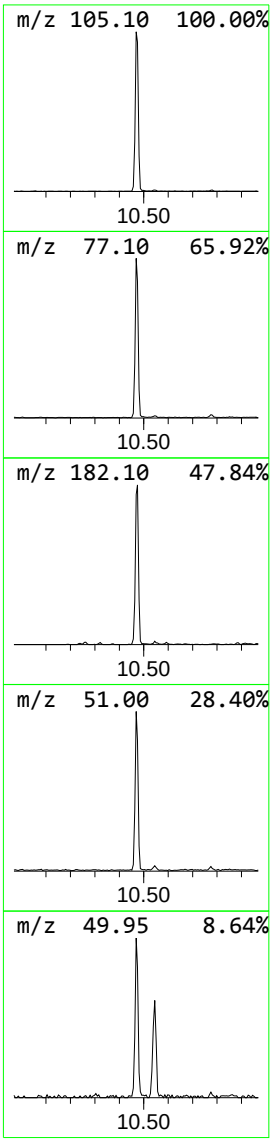
****

Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.469	6.83 ng	556370	Acenaphthene-d10	9.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzilamide	227	C14H13NO2	004746-87-6	50
3	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	49
4	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47
5	Ethanone, 2-bromo-1-phenyl-	198	C8H7BrO	000070-11-1	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
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Operator : CG\JU
Sample : 02616-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

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

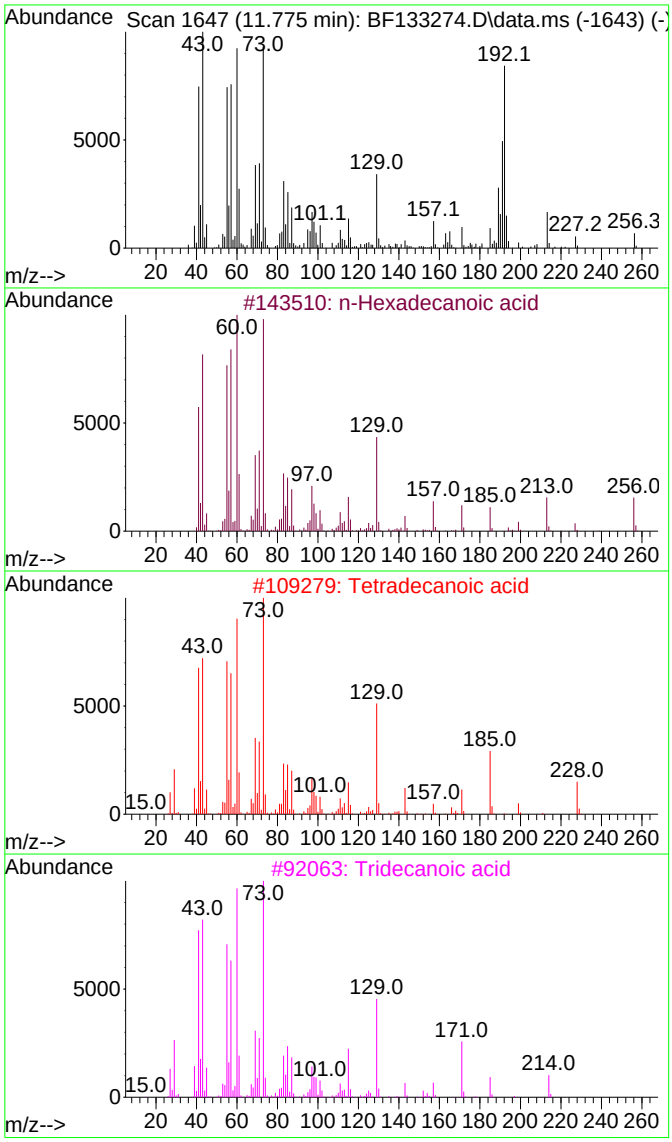
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

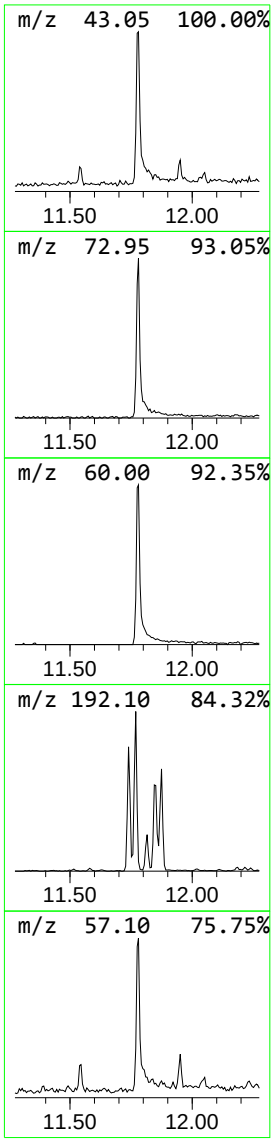
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.775	6.07 ng	504466	Phenanthrene-d10	11.239

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	70
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	55
5	Undecanoic acid	186	C11H22O2	000112-37-8	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133274.D
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Sample : 02616-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

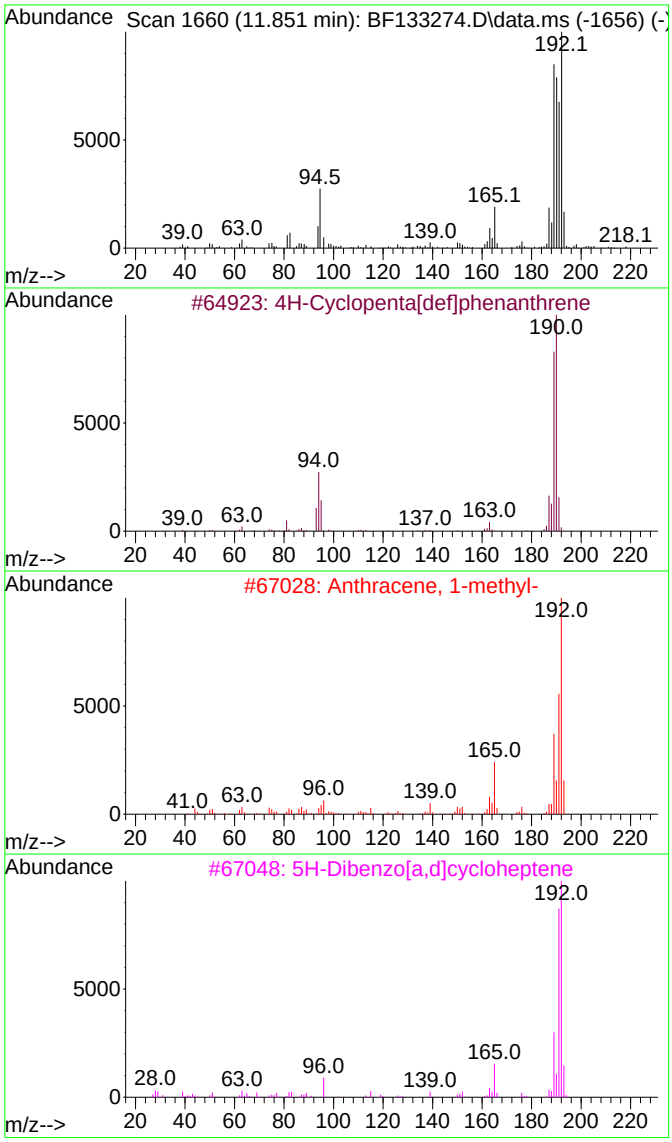
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

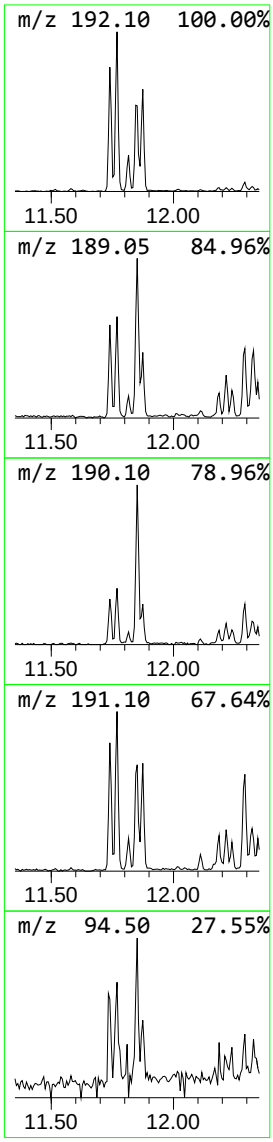
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.851	2.88 ng	239506	Phenanthrene-d10	11.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	53
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	52
3	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	46
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	46
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	42





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Sample : 02616-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

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

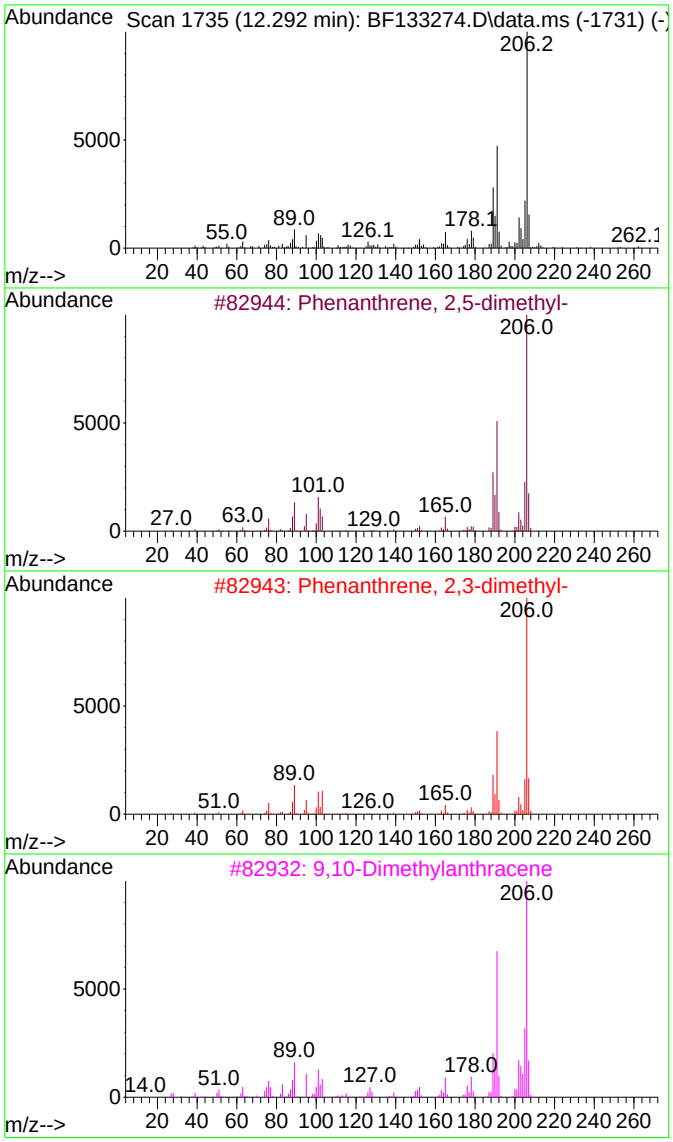
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

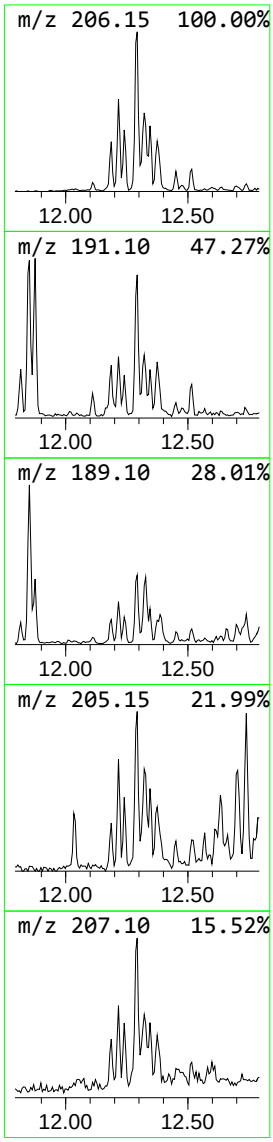
****

Peak Number 5 Phenanthrene, 2,5-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.292	2.45 ng	203966	Phenanthrene-d10	11.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	93
2	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	93
3	9,10-Dimethylanthracene	206	C16H14	000781-43-1	90
4	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	89
5	Phenanthrene, 2,7-dimethyl-	206	C16H14	001576-69-8	87





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Data File : BF133274.D
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Misc :
ALS Vial : 11 Sample Multiplier: 1

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

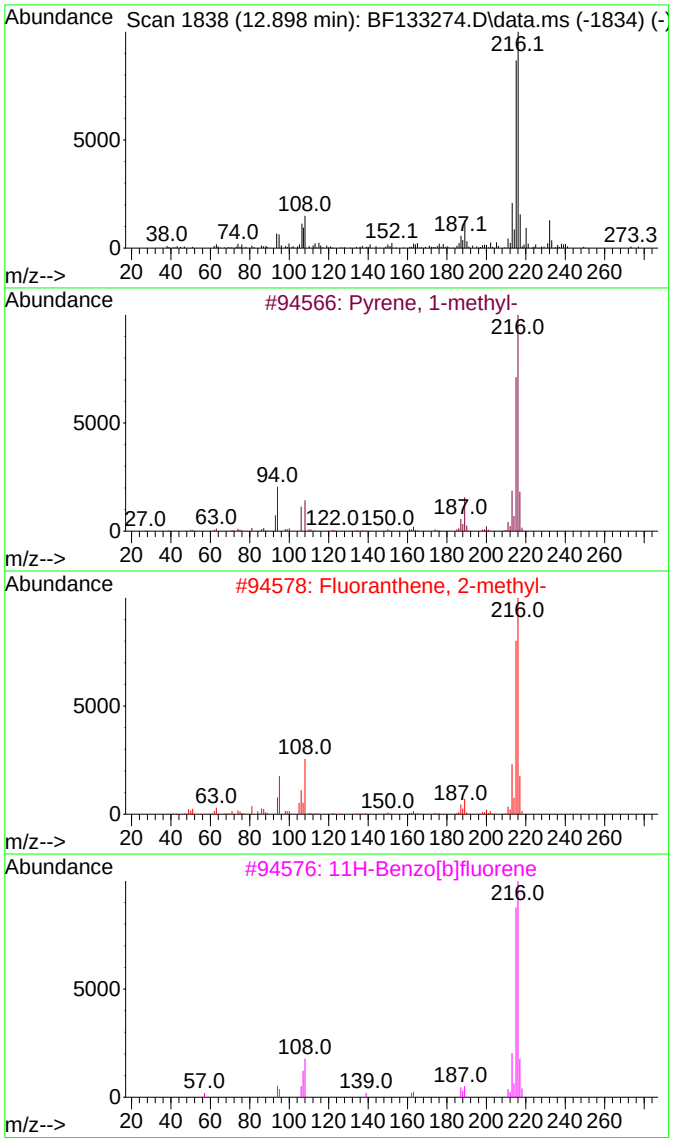
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

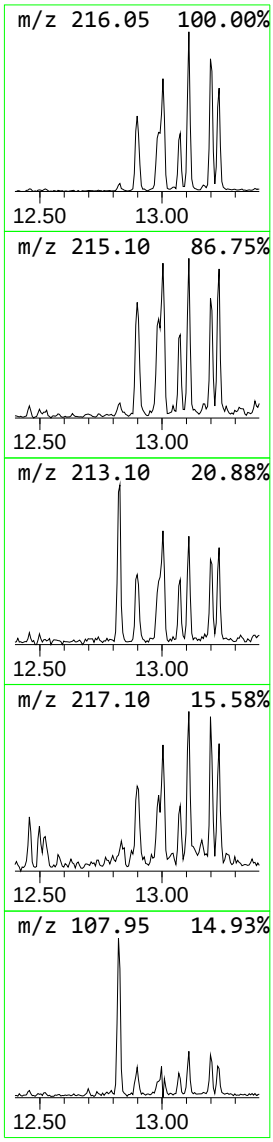
****

Peak Number 6 Pyrene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.898	2.08 ng	157952	Chrysene-d12	13.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
2	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	90
3	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	89
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	83
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133274.D
Acq On : 05 May 2023 20:50
Operator : CG\JU
Sample : 02616-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

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

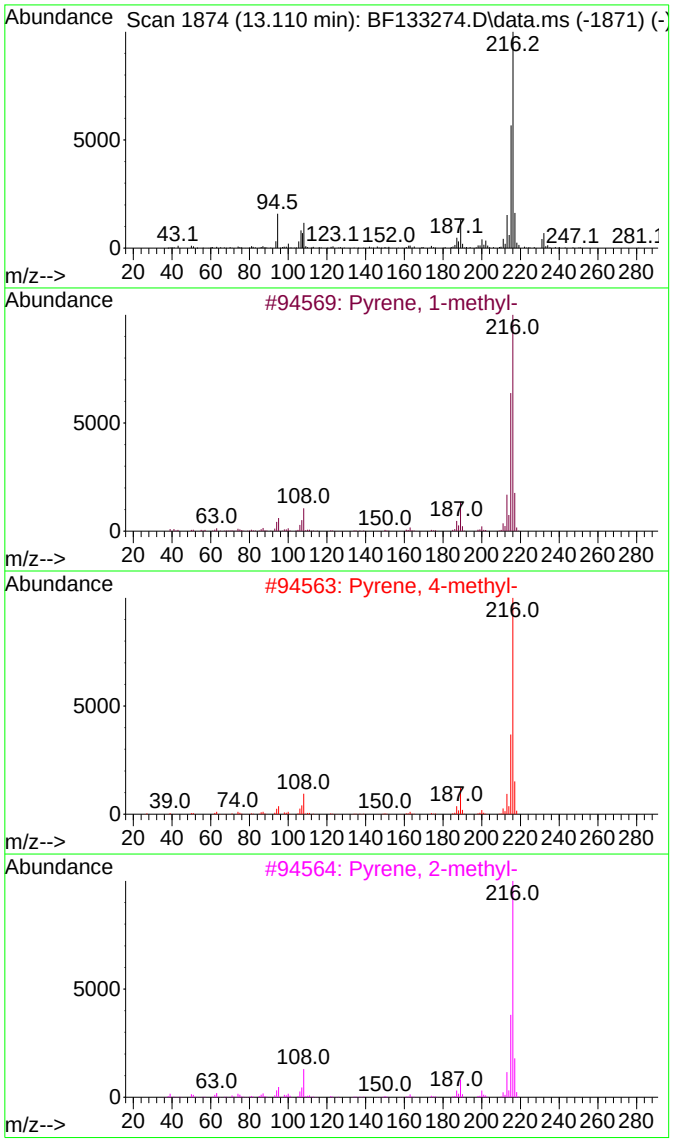
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

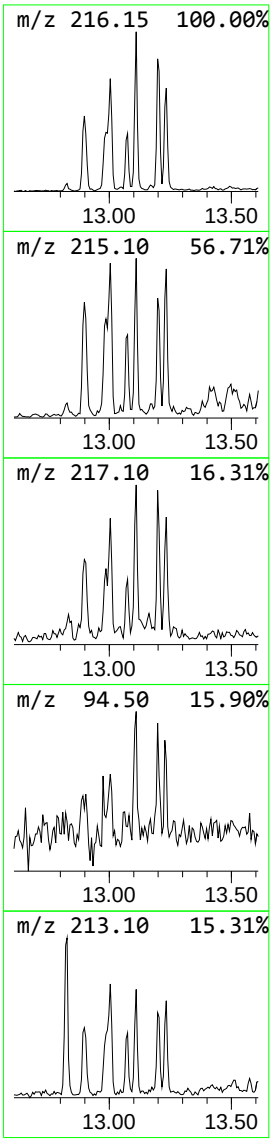
****

Peak Number 7 Pyrene, 4-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.110	2.01 ng	152797	Chrysene-d12	13.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	96
2	Pyrene, 4-methyl-	216	C17H12	003353-12-6	96
3	Pyrene, 2-methyl-	216	C17H12	003442-78-2	95
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	93
5	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90





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Data File : BF133274.D
Acq On : 05 May 2023 20:50
Operator : CG\JU
Sample : 02616-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

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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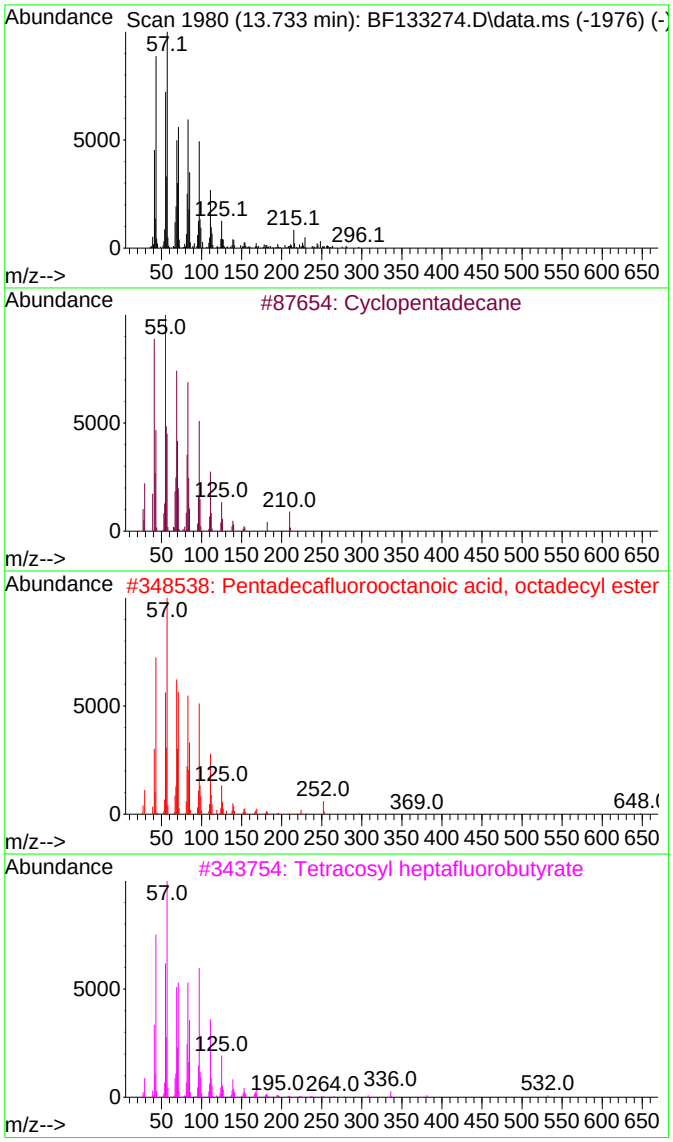
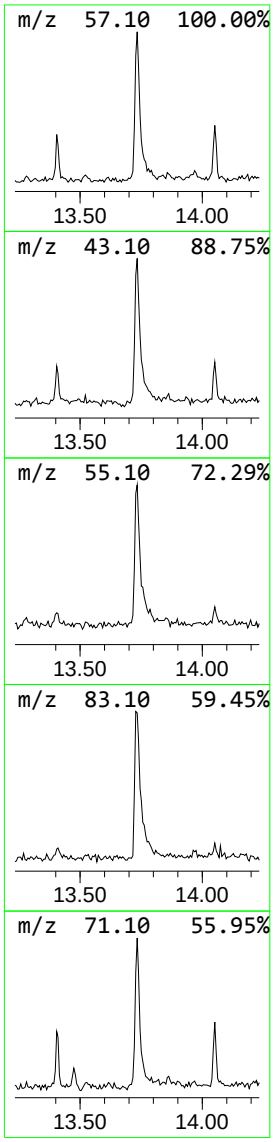
Peak Number 8 Cyclopentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.733	4.82 ng	366083	Chrysene-d12	13.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	97
2	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
3	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91





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Operator : CG\JU
Sample : 02616-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

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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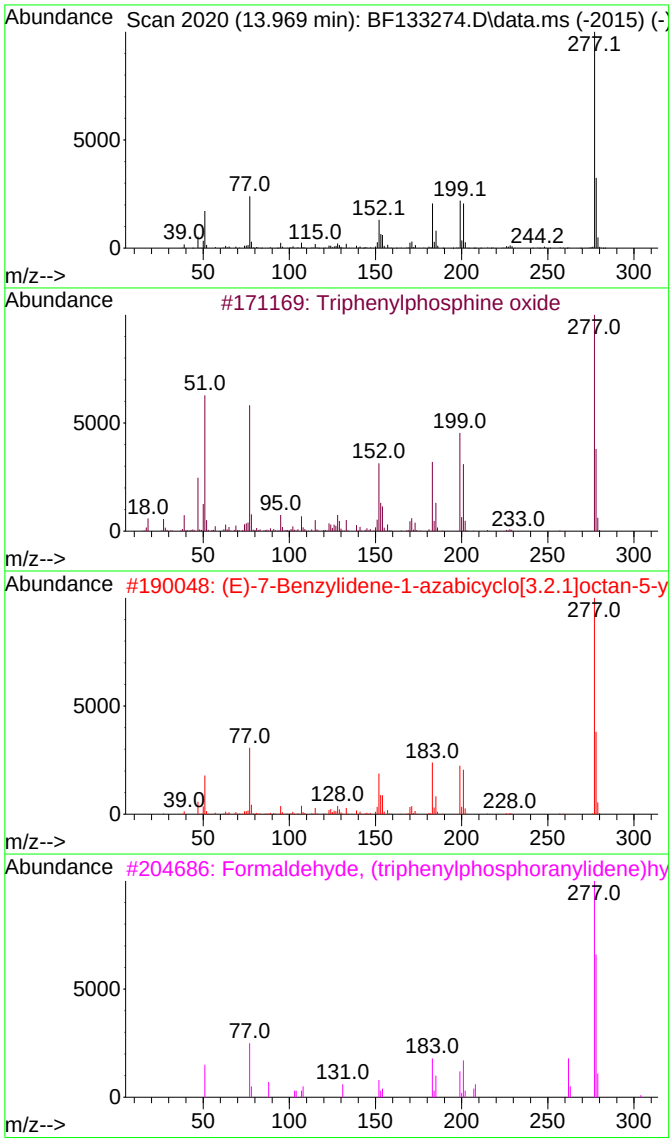
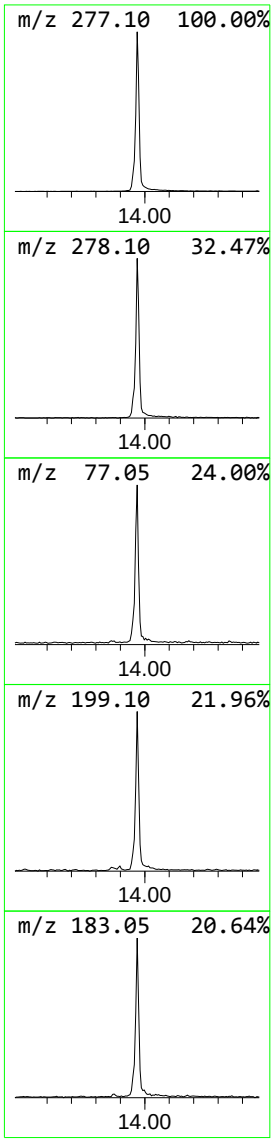
Peak Number 9 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.969	12.44 ng	944884	Chrysene-d12	13.874

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	83
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
4	Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	32
5	2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	32





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Data File : BF133274.D
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Operator : CG\JU
Sample : 02616-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

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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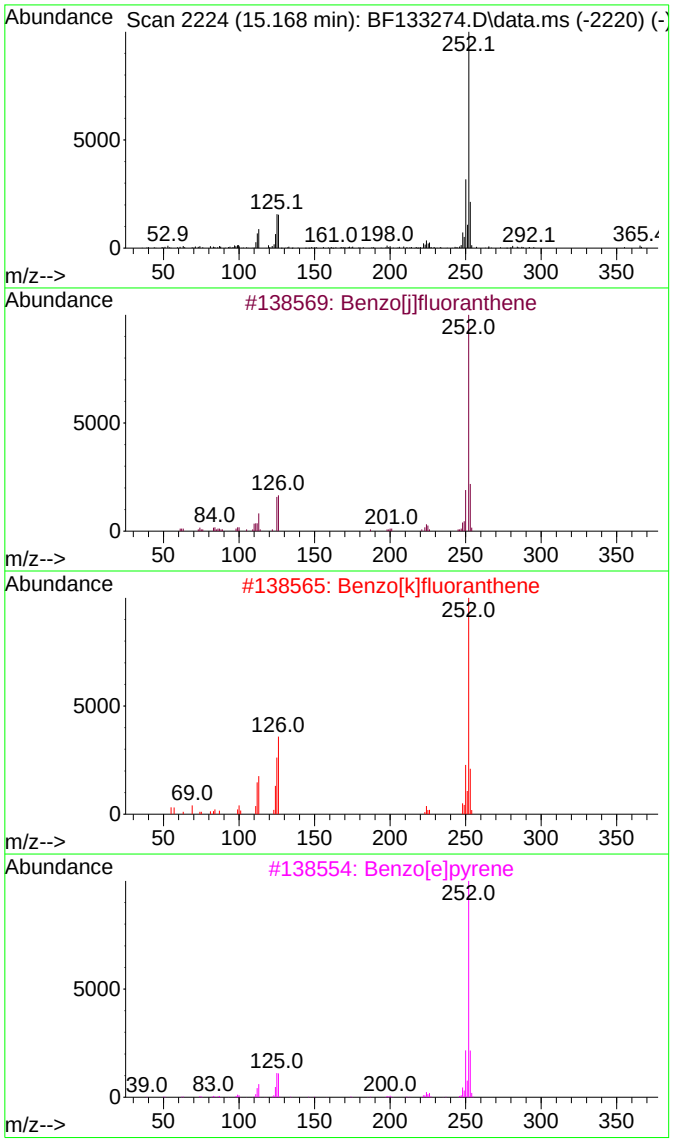
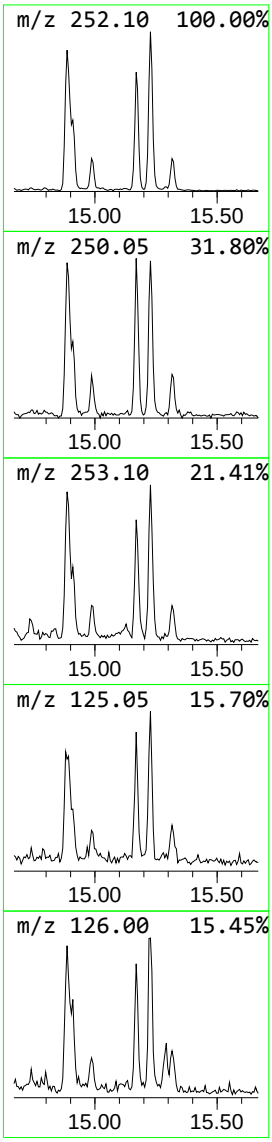
Peak Number 10 Benzo[j]fluoranthene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.169	2.43 ng	125385	Perylene-d12	15.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[j]fluoranthene	252	C20H12	000205-82-3	96
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
3	Benzo[e]pyrene	252	C20H12	000192-97-2	95
4	Benzo[a]pyrene	252	C20H12	000050-32-8	93
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93





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Operator : CG\JU
Sample : 02616-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

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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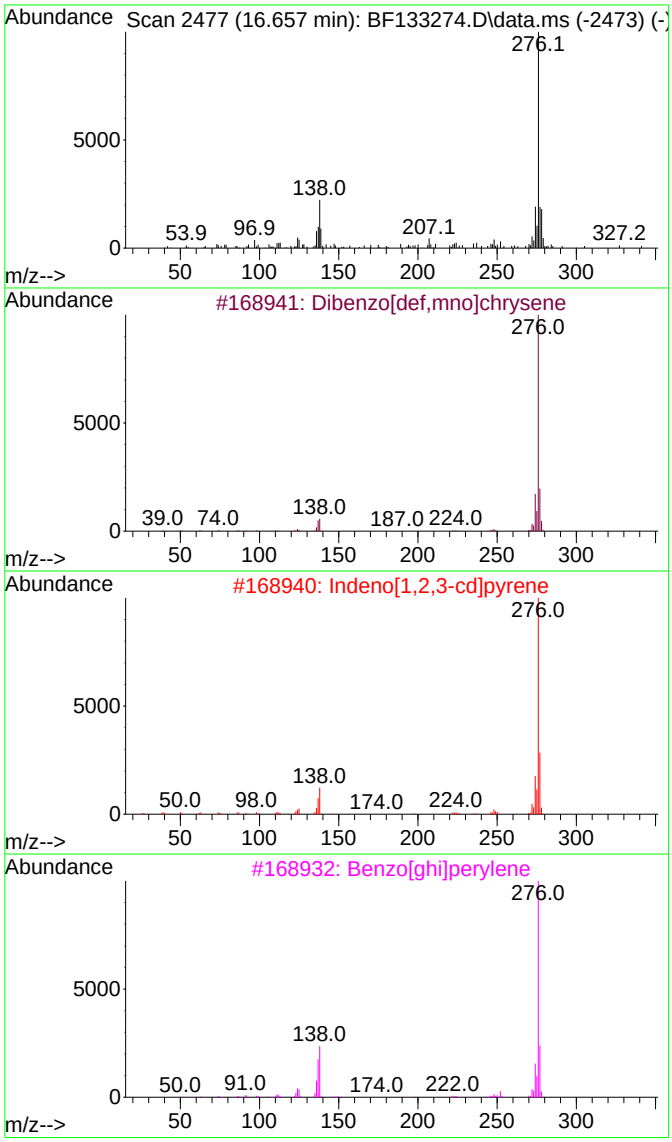
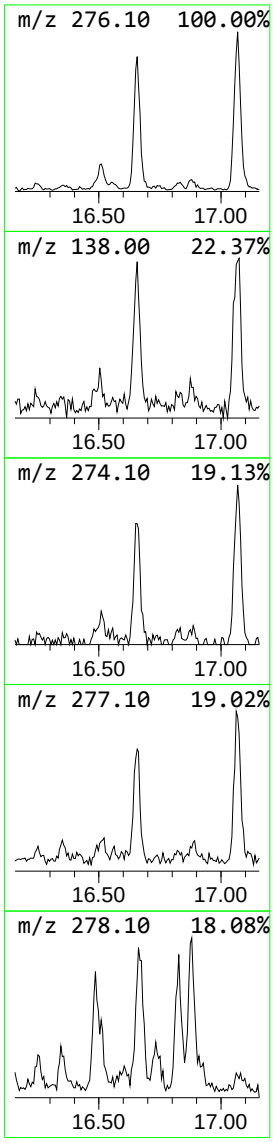
Peak Number 11 Dibenzo[def,mno]chrysene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.657	2.03 ng	104809	Perylene-d12	15.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	90
2	Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	90
3	Benzo[ghi]perylene	276	C22H12	000191-24-2	76
4	5,7-Dibromo-1H-indazole	274	C7H4Br2N2	050477-28-6	49
5	6H-Pyrido[4,3-b]carbazole, 9-met...	276	C18H16N2O	010371-86-5	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133274.D
Acq On : 05 May 2023 20:50
Operator : CG\JU
Sample : 02616-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

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-...	4.916	12.3	ng	676587	1	6.728	1100330	20.0
Benzophenone	10.469	6.8	ng	556370	3	9.757	1628290	20.0
n-Hexadecanoic ...	11.775	6.1	ng	504466	4	11.239	1663050	20.0
4H-Cyclopenta[d...	11.851	2.9	ng	239506	4	11.239	1663050	20.0
Phenanthrene, 2...	12.292	2.5	ng	203966	4	11.239	1663050	20.0
Pyrene, 1-methyl-	12.898	2.1	ng	157952	5	13.874	1519140	20.0
Pyrene, 4-methyl-	13.110	2.0	ng	152797	5	13.874	1519140	20.0
Cyclopentadecane	13.733	4.8	ng	366083	5	13.874	1519140	20.0
Triphenylphosph...	13.969	12.4	ng	944884	5	13.874	1519140	20.0
Benzo[j]fluoran...	15.169	2.4	ng	125385	6	15.292	1030150	20.0
Dibenzo[def,mno...	16.657	2.0	ng	104809	6	15.292	1030150	20.0