LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130976.D
Acq On : 04 Nov 2022 00:06
Operator : CG\JU
Sample : N5418-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-K

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-BF102722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130976.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	11	18	26	rVB	453745	580446	37.53%	4.077%
2	2.305	33	37	44	rBV	35936	47525	3.07%	0.334%
3	5.134	514	518	530	rVB	361830	405214	26.20%	2.846%
4	5.534	581	586	589	rBV	1666194	1469361	95.00%	10.320%
5	6.534	752	756	760	rBV	1410721	1392456	90.03%	9.779%
6	6.916	818	821	825	rBV	545097	433071	28.00%	3.042%
7	7.481	912	917	920	rBV	1033178	860731	55.65%	6.045%
8	8.204	1036	1040	1043	rBV	552379	480033	31.04%	3.371%
9	9.281	1219	1223	1226	rBV	1499291	1333415	86.21%	9.365%
10	9.686	1287	1292	1297	rVB3	11899	20596	1.33%	0.145%
11	9.822	1312	1315	1319	rBV	46412	41227	2.67%	0.290%
12	9.963	1335	1339	1342	rVB	636136	494269	31.96%	3.471%
13	10.510	1430	1432	1438	rVB3	18130	21329	1.38%	0.150%
14	10.751	1470	1473	1477	rBV	1080847	899817	58.18%	6.320%
15	10.875	1489	1494	1497	rVB3	27888	35186	2.27%	0.247%
16	11.063	1521	1526	1528	rBV2	15608	20340	1.32%	0.143%
17	11.351	1571	1575	1578	rVB2	20298	28779	1.86%	0.202%
18	11.457	1589	1593	1595	rBV	681053	558231	36.09%	3.921%
19	11.480	1595	1597	1601	rVV	146474	112813	7.29%	0.792%
20	11.528	1601	1605	1608	rVV	51781	54749	3.54%	0.385%
21	11.563	1608	1611	1614	rBV2	19365	19178	1.24%	0.135%
22	11.739	1637	1641	1647	rBV7	12444	24597	1.59%	0.173%
23	11.786	1647	1649	1653	rVB	26081	21325	1.38%	0.150%
24	11.839	1654	1658	1661	rBV	44998	38532	2.49%	0.271%
25	11.957	1675	1678	1681	rBV	64919	66671	4.31%	0.468%
26	11.986	1681	1683	1686	rVV	77513	58213	3.76%	0.409%
27	12.033	1688	1691	1694	rVV	32977	30229	1.95%	0.212%
28	12.069	1694	1697	1700	rVV2	90816	112276	7.26%	0.789%
29	12.092	1700	1701	1708	rVB	59946	41520	2.68%	0.292%
30	12.257	1726	1729	1731	rBV	34979	33184	2.15%	0.233%
31	12.386	1748	1751	1752	rBV	19996	19666	1.27%	0.138%
32	12.433	1757	1759	1761	rBV	36692	27698	1.79%	0.195%
33	12.510	1769	1772	1774	rBV	88669	83552	5.40%	0.587%
34	12.545	1774	1778	1780	rVV3	54986	73769	4.77%	0.518%
35	12.563	1780	1781	1784	rVB	28081	20128	1.30%	0.141%
36	12.598	1784	1787	1791	rBV3	33228	49403	3.19%	0.347%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130976.D
Acq On : 04 Nov 2022 00:06
Operator : CG\JU
Sample : N5418-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-K

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-BF102722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.675	1796	1800	1803	rBV	284959	246159	15.92%	1.729%
38	12.904	1833	1839	1845	rBV	344327	383733	24.81%	2.695%
39	12.957	1845	1848	1852	rVB2	43815	48267	3.12%	0.339%
40	13.045	1859	1863	1866	rBV	1868417	1546649	100.00%	10.862%
41	13.116	1872	1875	1883	rBV4	51100	92555	5.98%	0.650%
42	13.210	1888	1891	1892	rVV2	44451	46896	3.03%	0.329%
43	13.233	1892	1895	1898	rVB	79602	85560	5.53%	0.601%
44	13.298	1904	1906	1909	rBV	55869	41694	2.70%	0.293%
45	13.339	1910	1913	1915	rBV3	76397	69380	4.49%	0.487%
46	13.427	1926	1928	1931	rBV	58995	53720	3.47%	0.377%
47	13.463	1931	1934	1937	rVV	52961	52856	3.42%	0.371%
48	13.610	1957	1959	1961	rBV	31688	28714	1.86%	0.202%
49	14.104	2039	2043	2046	rBV2	635204	703740	45.50%	4.942%
50	14.133	2046	2048	2054	rVB	144051	128583	8.31%	0.903%
51	14.198	2056	2059	2063	rVB	173922	179786	11.62%	1.263%
52	14.868	2171	2173	2175	rBV	71038	65779	4.25%	0.462%
53	15.615	2297	2300	2311	rVB	289773	455030	29.42%	3.196%

Sum of corrected areas: 14238630

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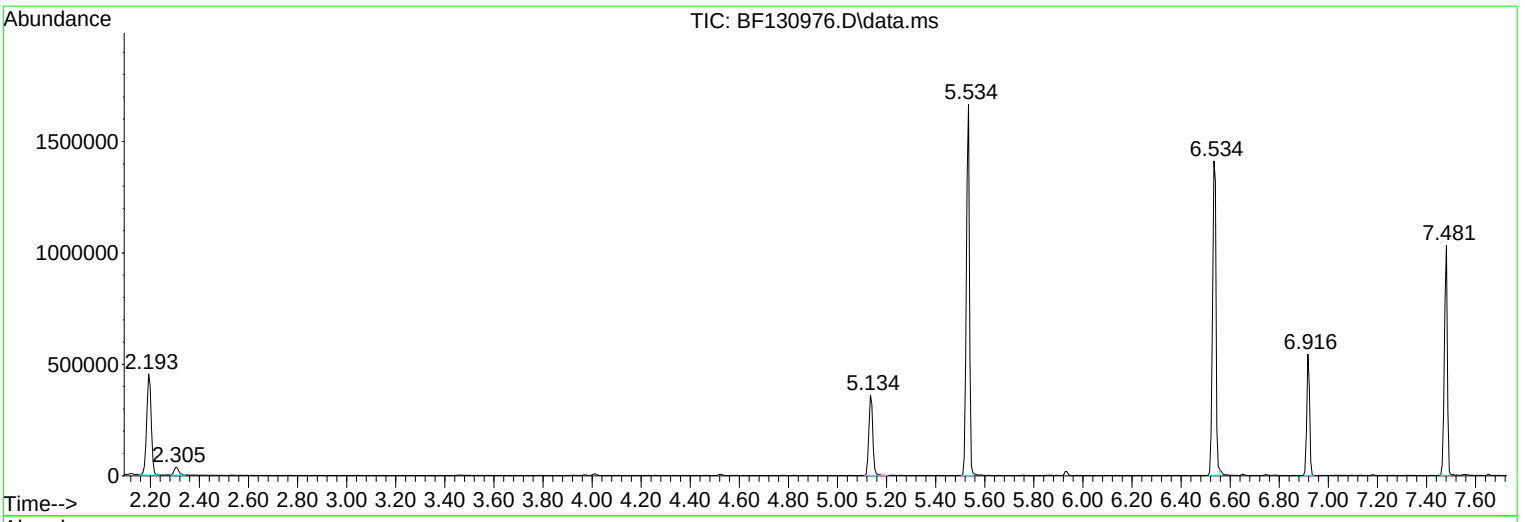
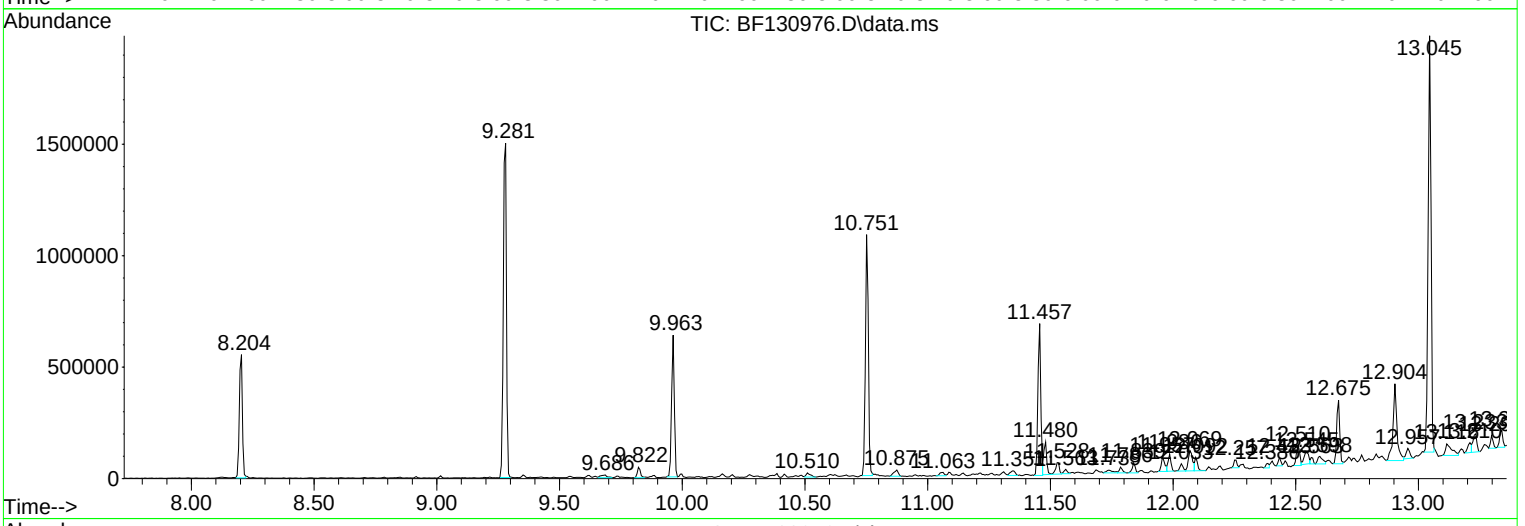
Misc :
ALS Vial : 13 Sample Multiplier: 1

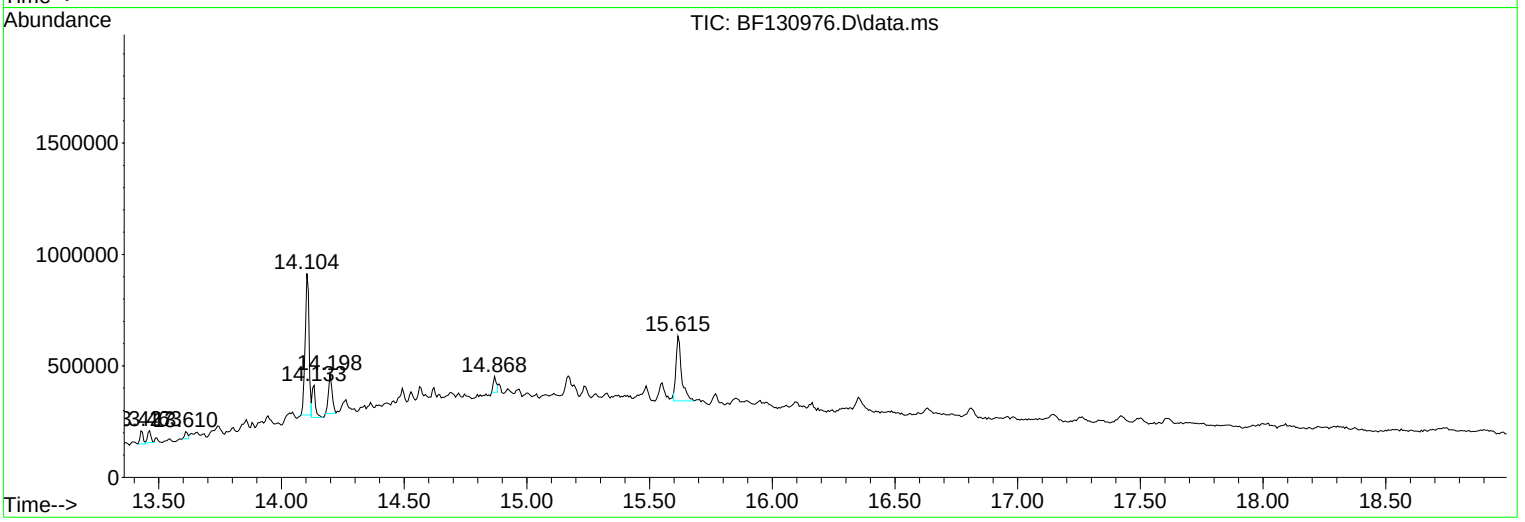
Instrument :
BNA_F
ClientSampleId :
TP-K

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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\BF110322\
Data File : BF130976.D
Acq On : 04 Nov 2022 00:06
Operator : CG\JU
Sample : N5418-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-K

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

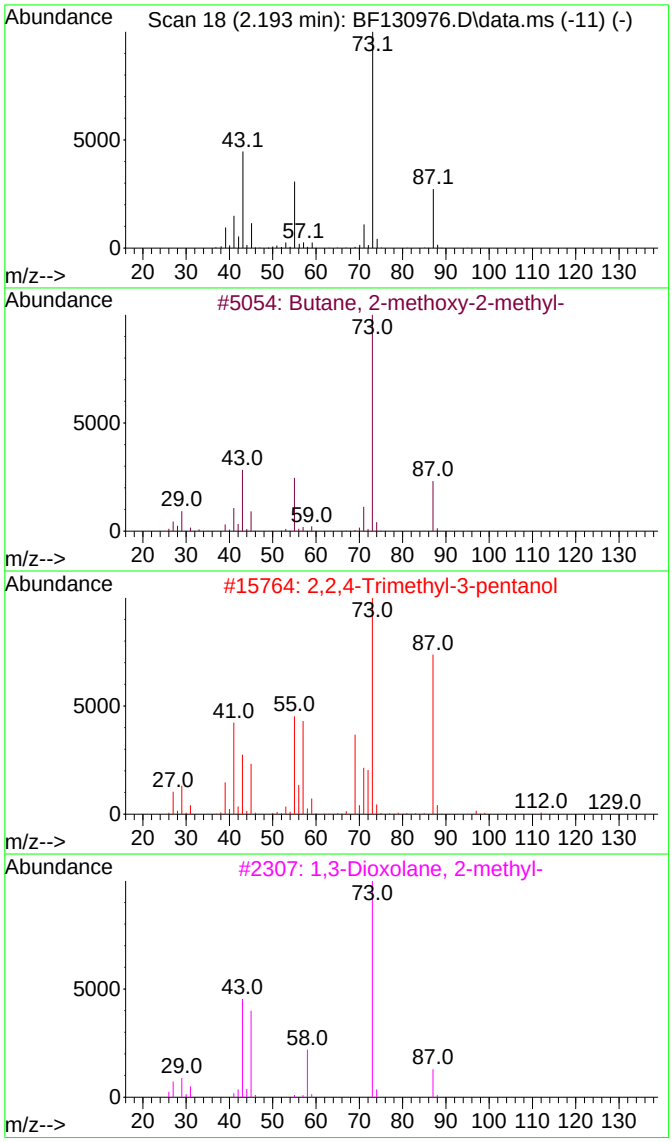
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

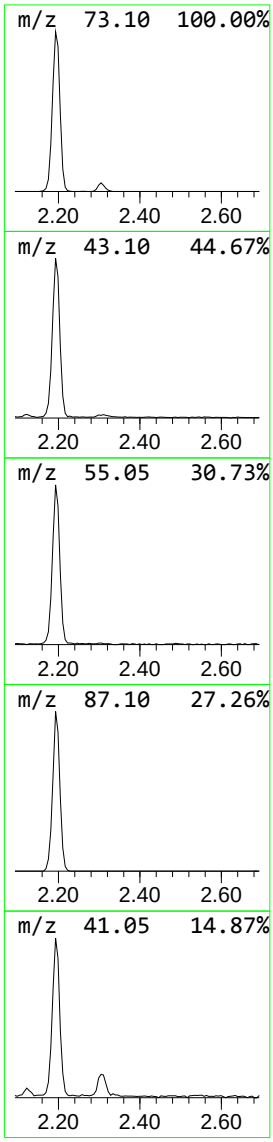
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	26.81 ng	580446	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130976.D
Acq On : 04 Nov 2022 00:06
Operator : CG\JU
Sample : N5418-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-K

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

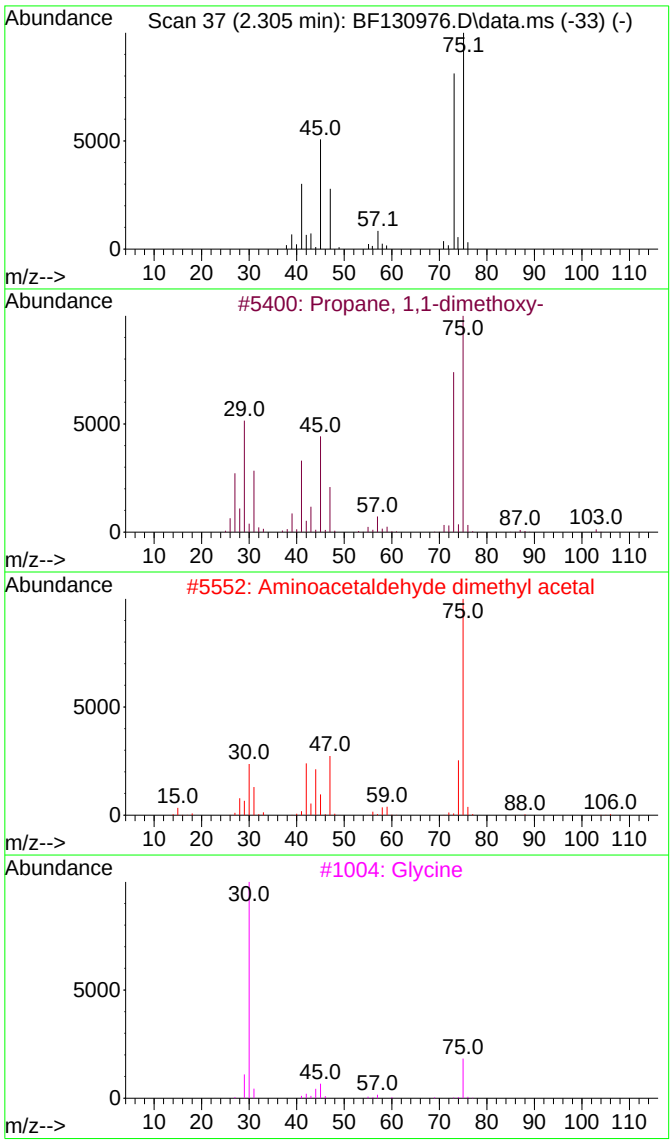
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

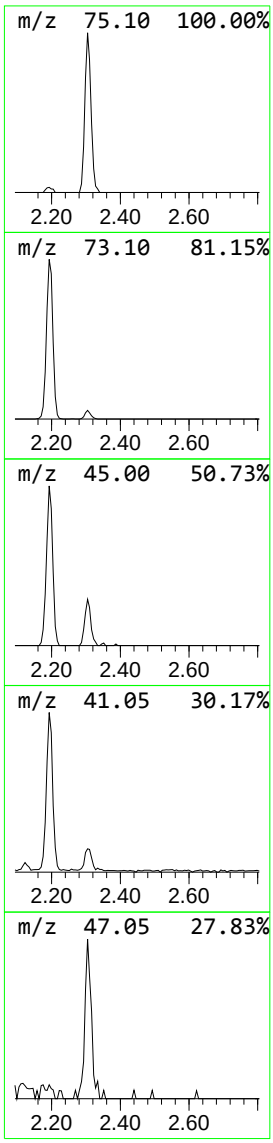
****

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.305	2.19 ng	47525	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2	Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	28
3	Glycine	75	C2H5NO2	000056-40-6	9
4	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9
5	1,3-Dioxolane, 2-(1,1-dimethylet...	130	C7H14O2	002568-29-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130976.D
Acq On : 04 Nov 2022 00:06
Operator : CG\JU
Sample : N5418-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-K

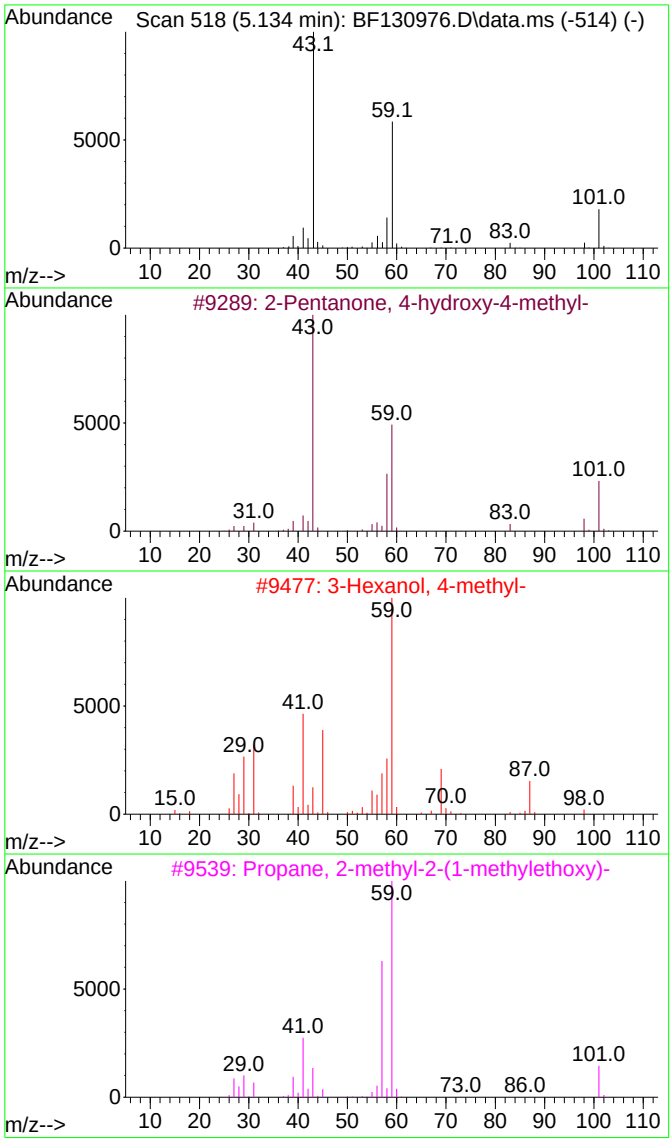
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

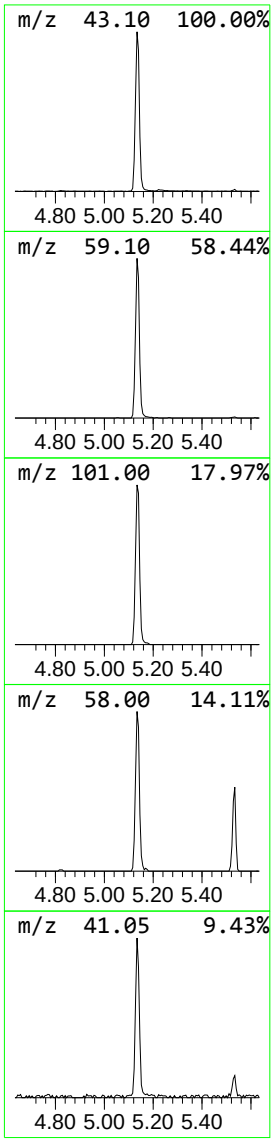
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.134	18.71 ng	405214	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130976.D
Acq On : 04 Nov 2022 00:06
Operator : CG\JU
Sample : N5418-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-K

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

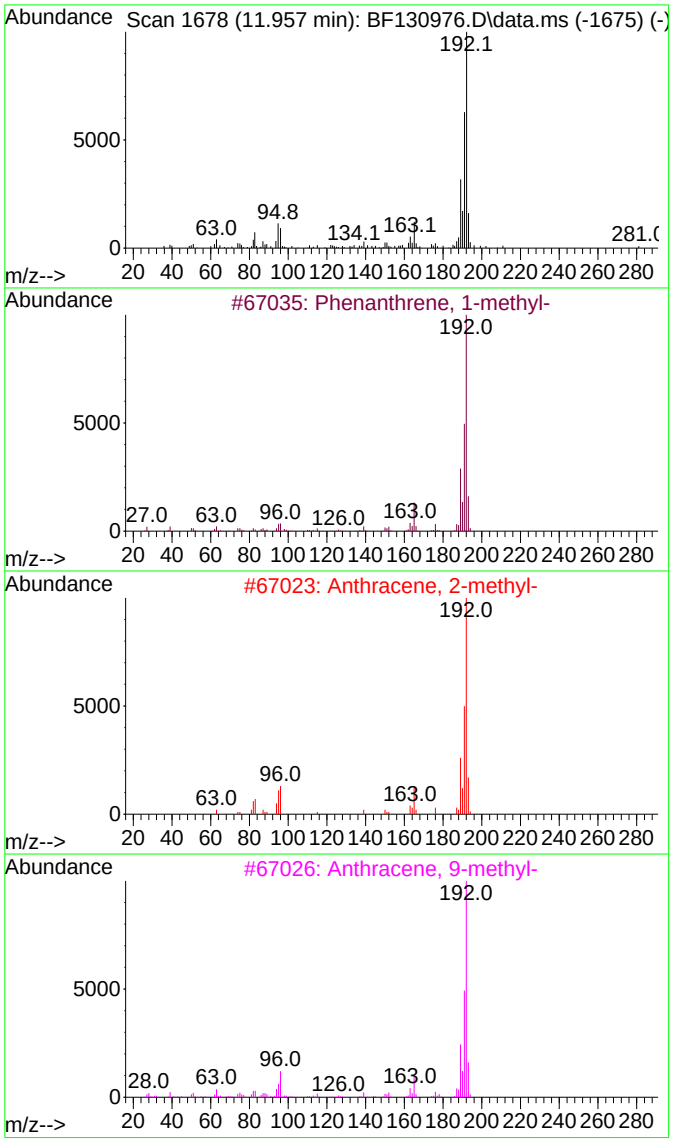
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

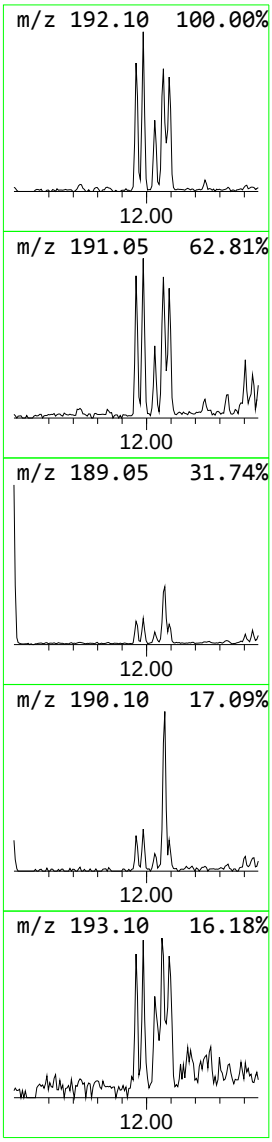
****

Peak Number 4 Phenanthrene, 1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	2.39 ng	66671	Phenanthrene-d10	11.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	90
4	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	90
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130976.D
Acq On : 04 Nov 2022 00:06
Operator : CG\JU
Sample : N5418-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-K

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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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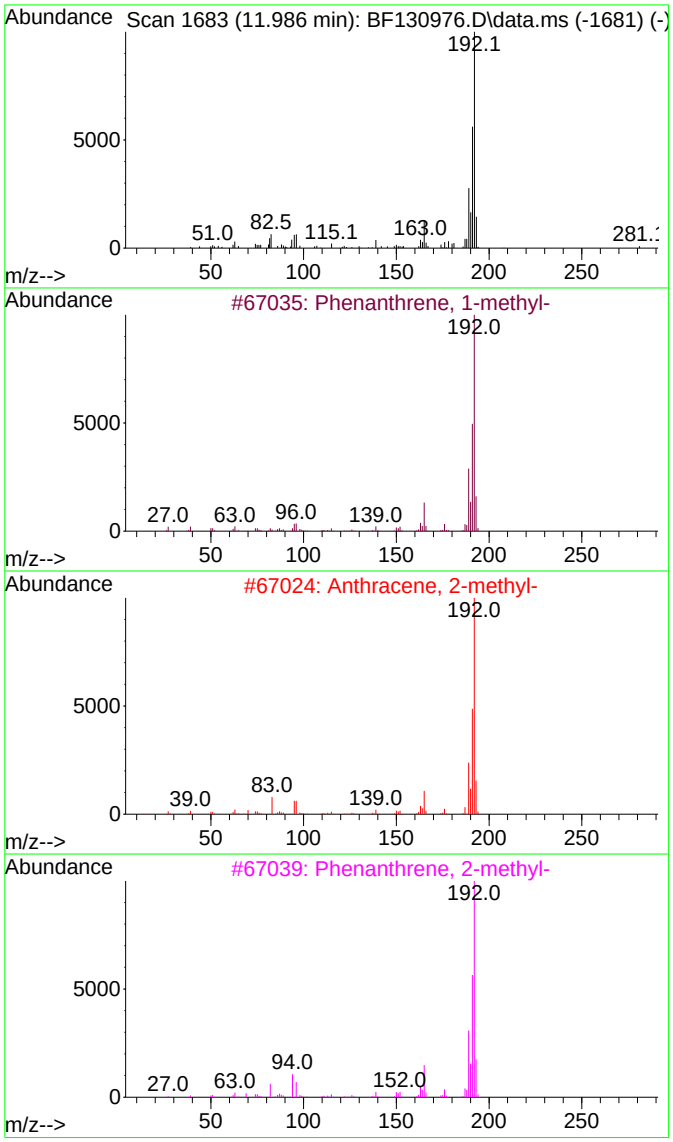
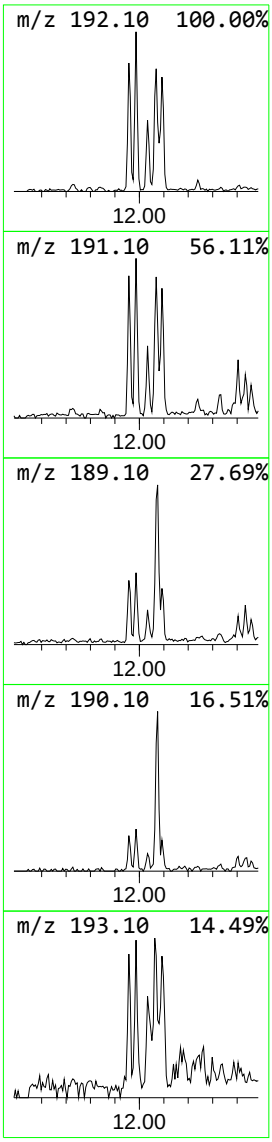
Peak Number 5 Anthracene, 2-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.986	2.09 ng	58213	Phenanthrene-d10	11.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	95
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	94
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	87
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
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Operator : CG\JU
Sample : N5418-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-K

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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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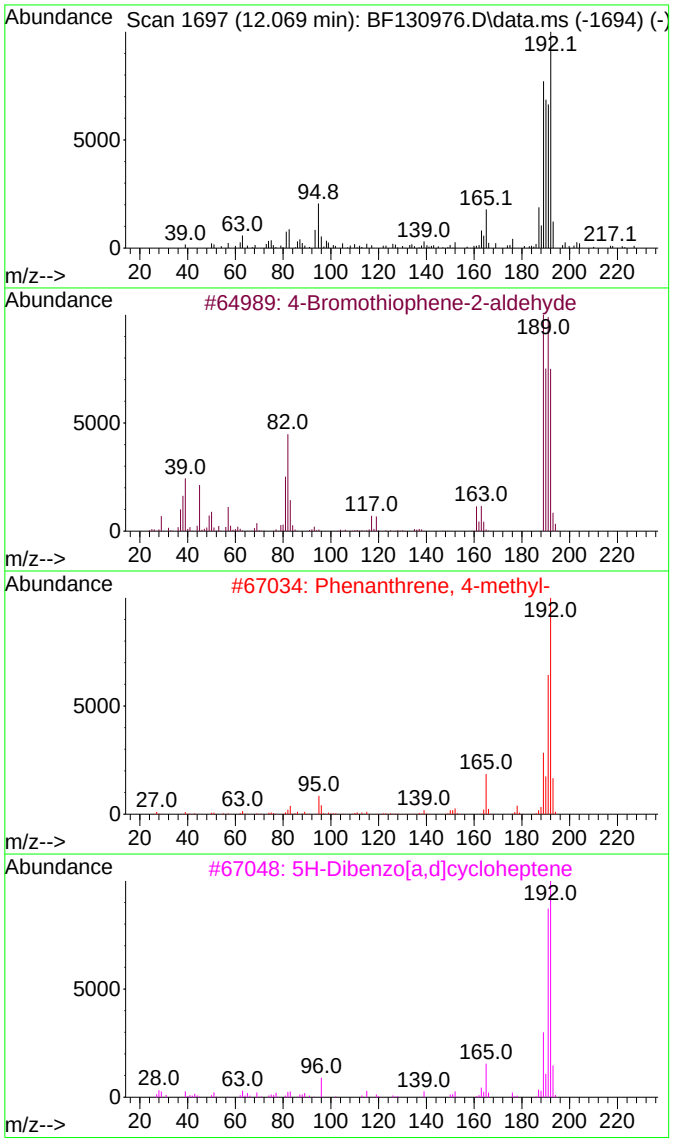
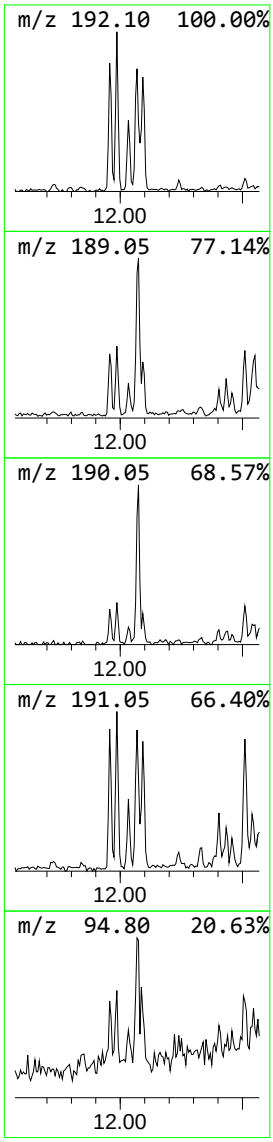
Peak Number 6 4-Bromothiophene-2-aldehyde Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.069	4.02 ng	112276	Phenanthrene-d10	11.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Bromothiophene-2-aldehyde	190	C5H3BrOS	018791-75-8	58
2	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	45
3	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	45
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	45
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130976.D
Acq On : 04 Nov 2022 00:06
Operator : CG\JU
Sample : N5418-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-K

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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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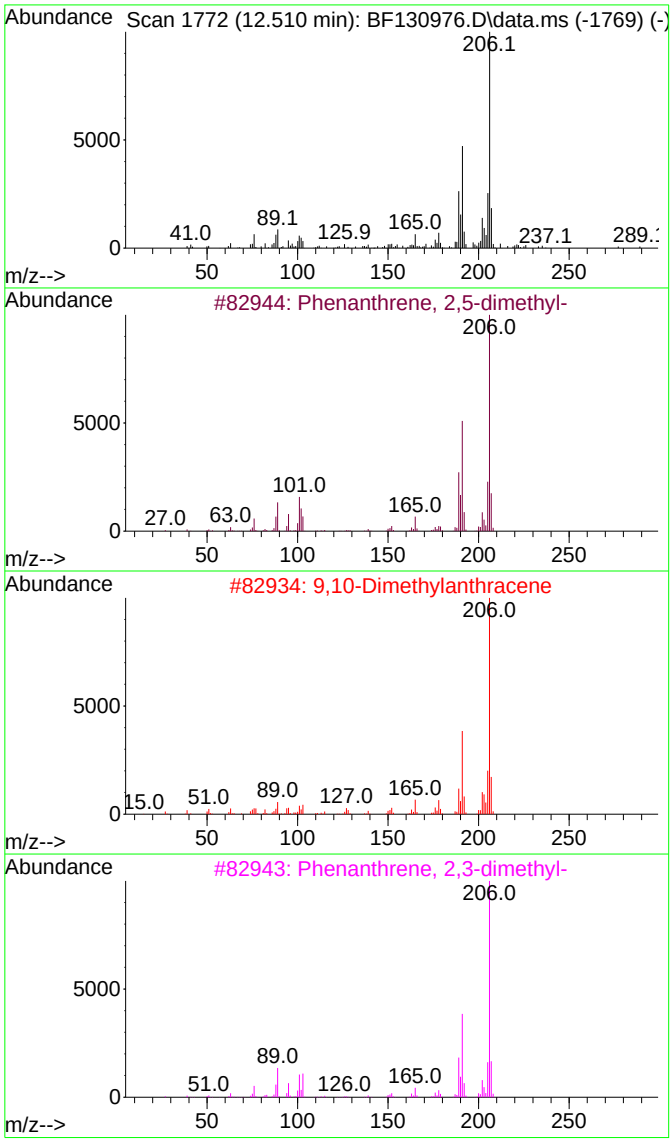
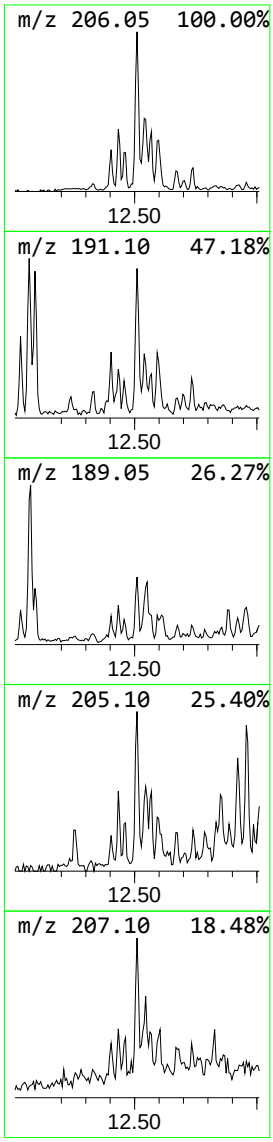
Peak Number 7 Phenanthrene, 2,5-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.510	2.99 ng	83552	Phenanthrene-d10	11.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	93
2	9,10-Dimethylanthracene	206	C16H14	000781-43-1	92
3	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	87
4	di-p-Tolylacetylene	206	C16H14	002789-88-0	87
5	3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130976.D
Acq On : 04 Nov 2022 00:06
Operator : CG\JU
Sample : N5418-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-K

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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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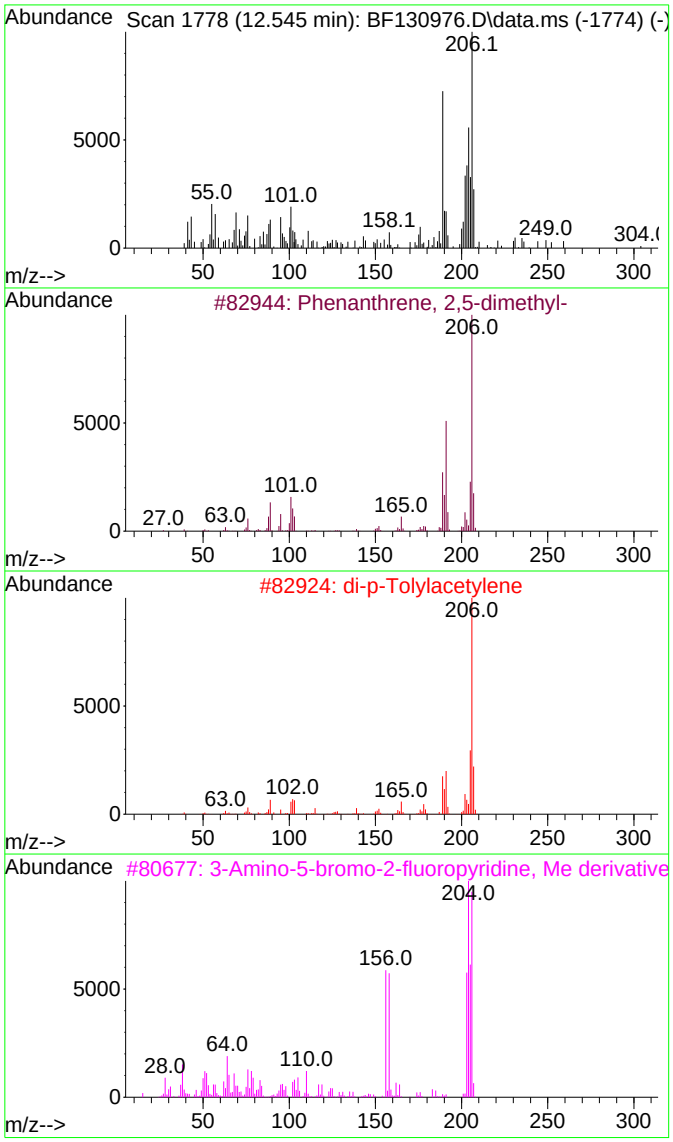
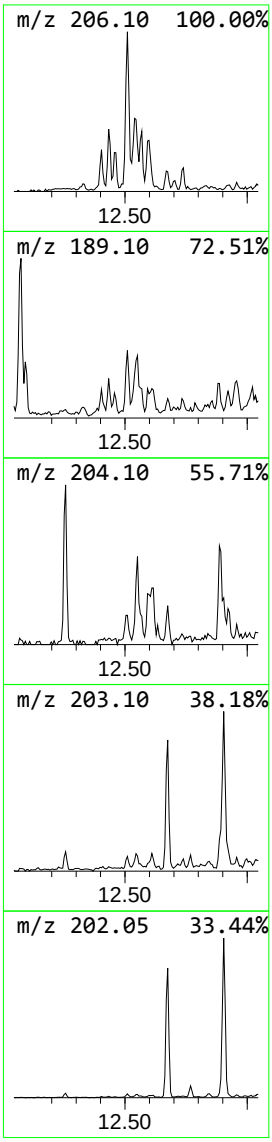
Peak Number 8 unknown12.545 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.545	2.64 ng	73769	Phenanthrene-d10	11.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	45
2	di-p-Tolylacetylene	206	C16H14	002789-88-0	43
3	3-Amino-5-bromo-2-fluoropyridine...	204	C6H6BrFN2	1000496-58-8	43
4	Pyrene, 4,5,9,10-tetrahydro-	206	C16H14	000781-17-9	41
5	Naphthalene, 1-phenyl-	204	C16H12	000605-02-7	38





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Data File : BF130976.D
Acq On : 04 Nov 2022 00:06
Operator : CG\JU
Sample : N5418-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-K

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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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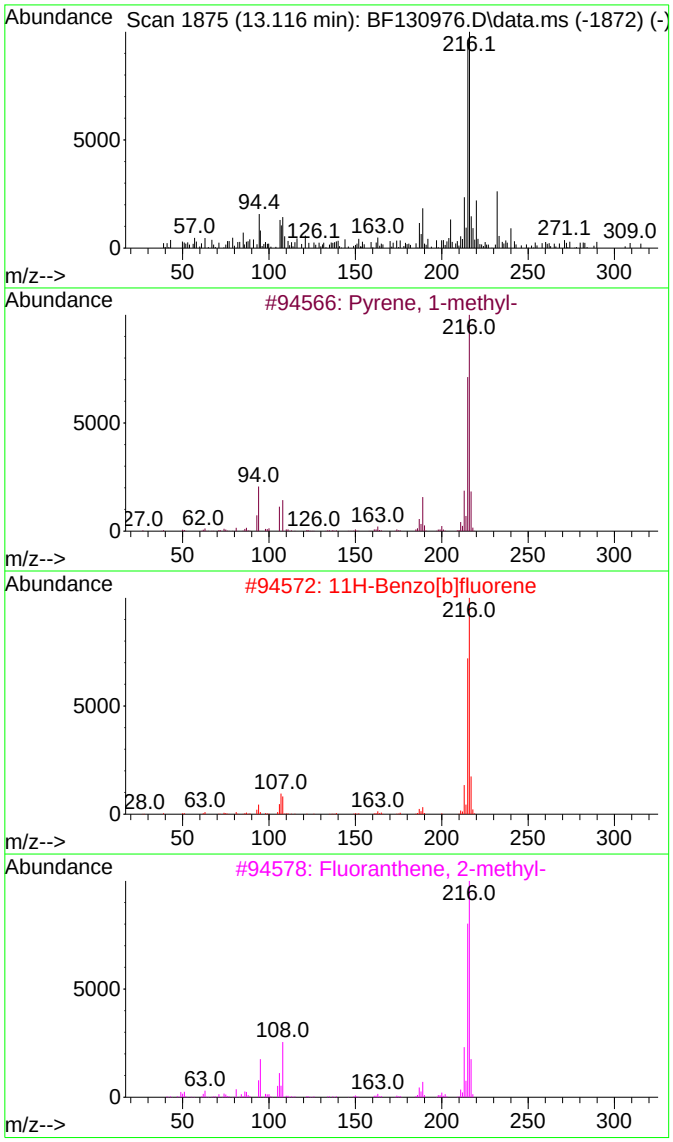
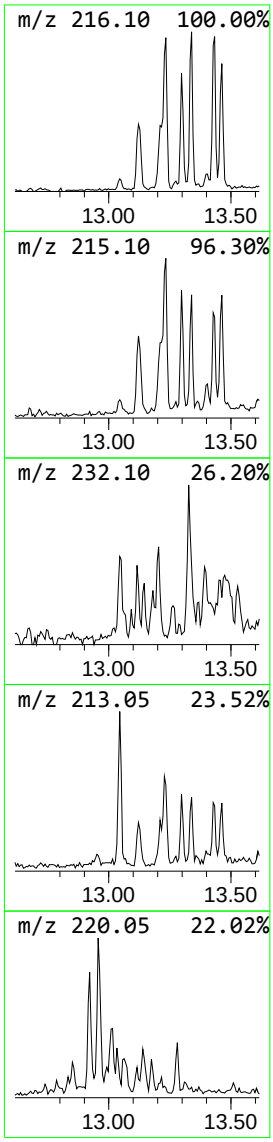
Peak Number 9 Pyrene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.116	2.63 ng	92555	Chrysene-d12	14.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	83
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	68
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	64
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	62
5	Pyrene, 2-methyl-	216	C17H12	003442-78-2	55





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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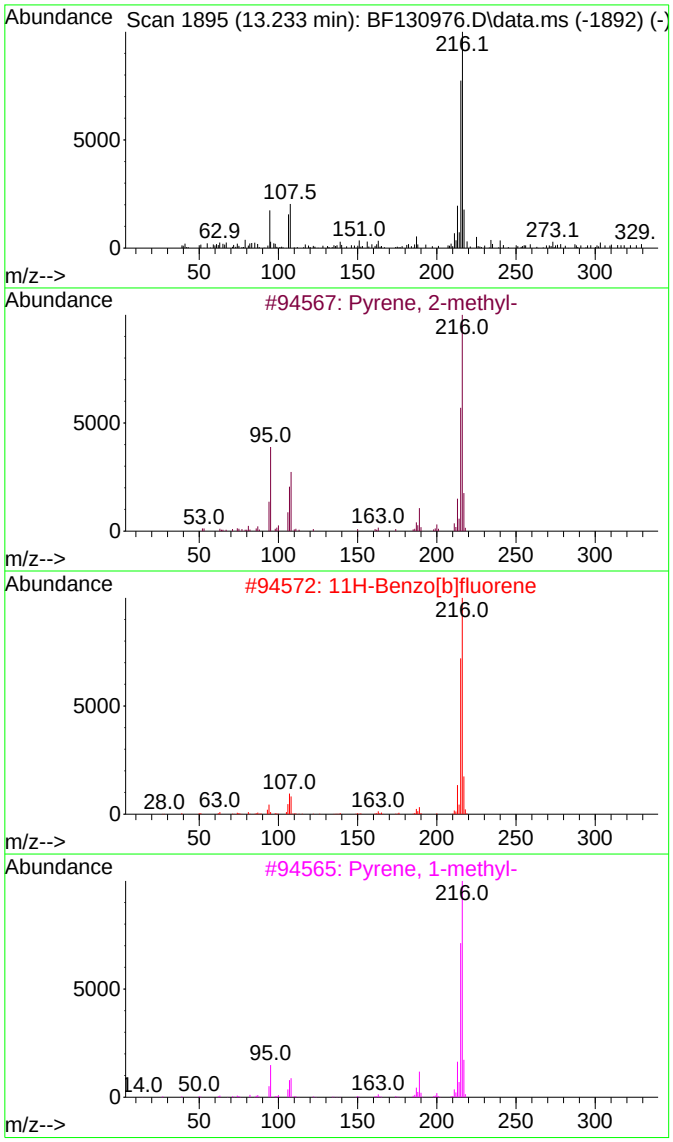
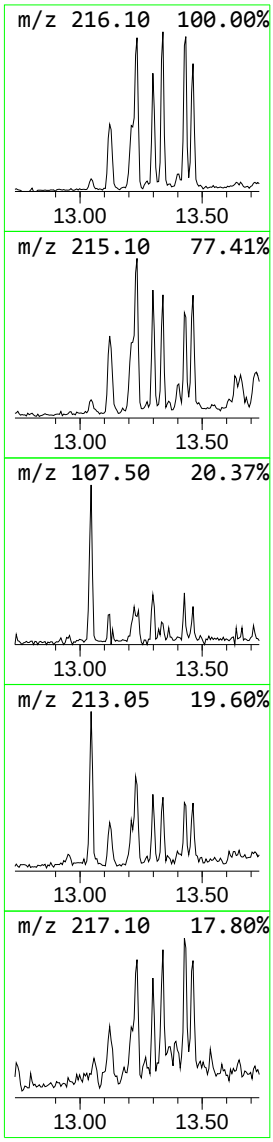
Peak Number 10 Pyrene, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.233	2.43 ng	85560	Chrysene-d12	14.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 2-methyl-	216	C17H12	003442-78-2	94
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
3	Pyrene, 1-methyl-	216	C17H12	002381-21-7	87
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	74
5	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	72





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Operator : CG\JU
Sample : N5418-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-K

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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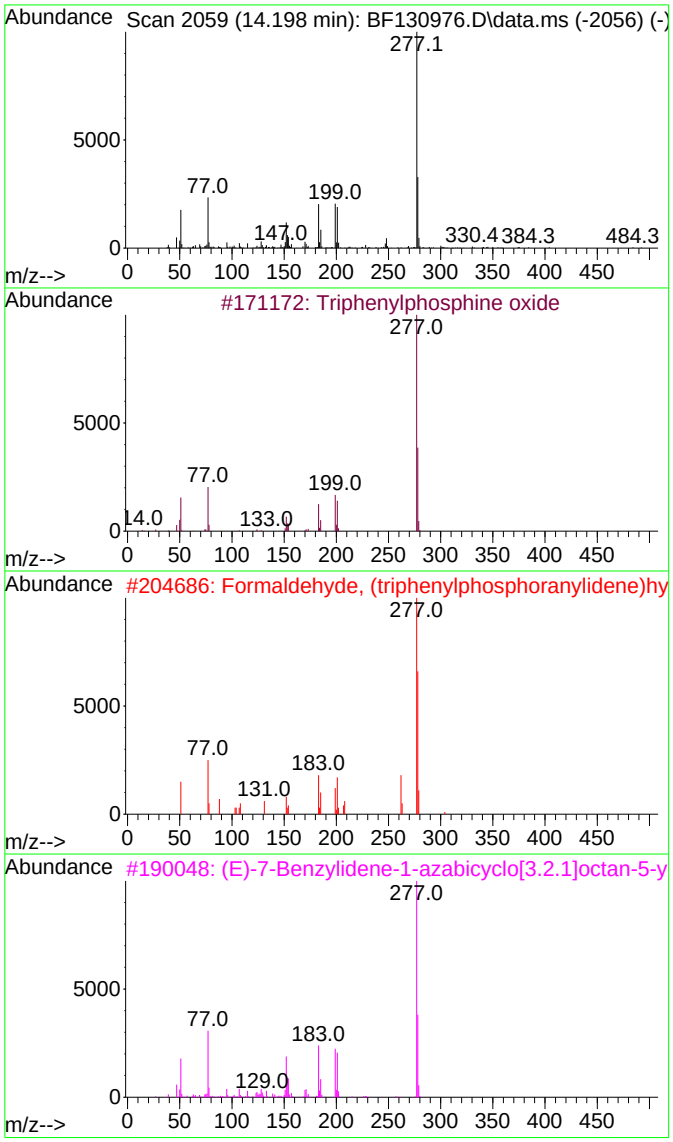
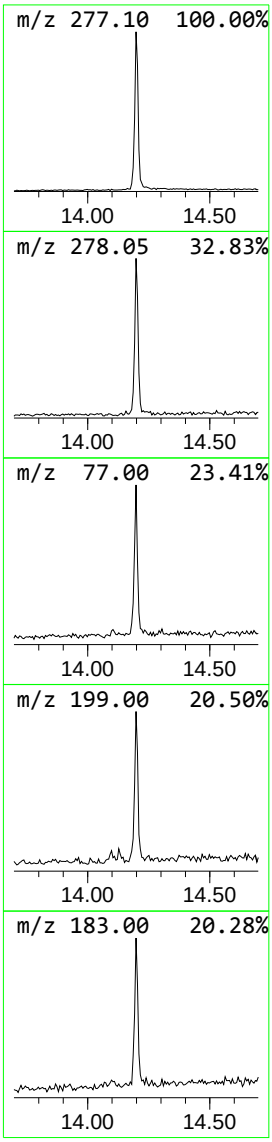
Peak Number 11 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.198	5.11 ng	179786	Chrysene-d12	14.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	59
3	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	52
4	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	38
5	Phenol, 2-(2,2-difluoro-1,3-benz...	277	C14H9F2NO3	1000274-10-8	28





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Operator : CG\JU
Sample : N5418-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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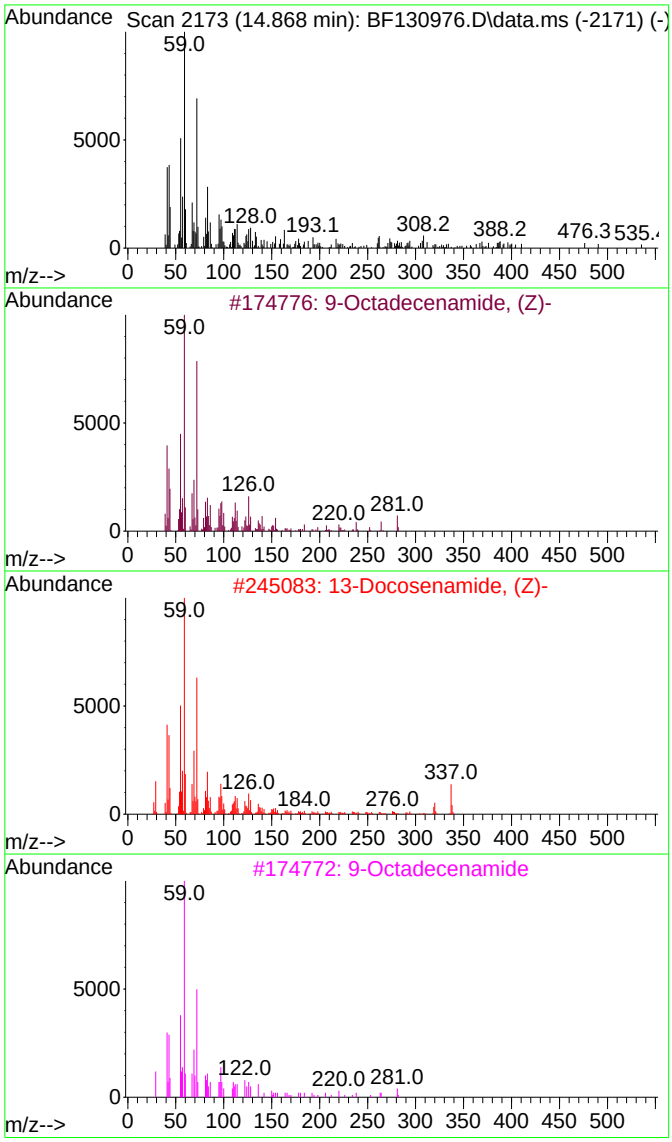
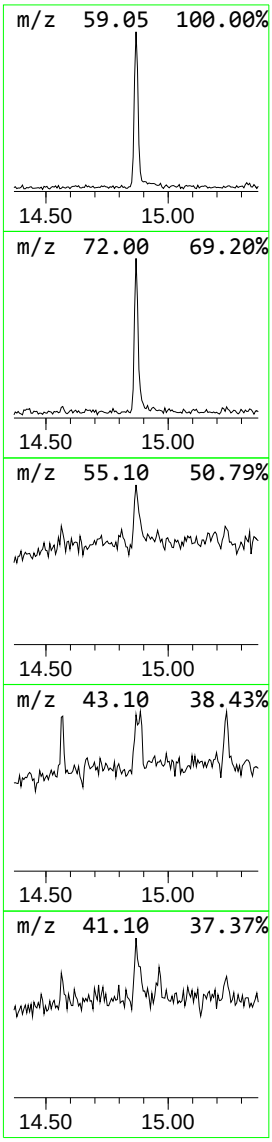
Peak Number 12 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.868	2.89 ng	65779	Perylene-d12	15.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	87
3	9-Octadecenamide	281	C18H35NO	003322-62-1	80
4	7-Nonenamide	155	C9H17NO	090949-53-4	64
5	Octadecanamide	283	C18H37NO	000124-26-5	53





Tentatively Identified Compound (LSC) summary

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Data File : BF130976.D
Acq On : 04 Nov 2022 00:06
Operator : CG\JU
Sample : N5418-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-K

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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...	2.193	26.8	ng	580446	1	6.916	433071	20.0
Propane, 1,1-di...	2.305	2.2	ng	47525	1	6.916	433071	20.0
2-Pentanone, 4-...	5.134	18.7	ng	405214	1	6.916	433071	20.0
Phenanthrene, 1...	11.957	2.4	ng	66671	4	11.457	558231	20.0
Anthracene, 2-m...	11.986	2.1	ng	58213	4	11.457	558231	20.0
4-Bromothiophen...	12.069	4.0	ng	112276	4	11.457	558231	20.0
Phenanthrene, 2...	12.510	3.0	ng	83552	4	11.457	558231	20.0
unknown12.545	12.545	2.6	ng	73769	4	11.457	558231	20.0
Pyrene, 1-methyl-	13.116	2.6	ng	92555	5	14.104	703740	20.0
Pyrene, 2-methyl-	13.233	2.4	ng	85560	5	14.104	703740	20.0
Triphenylphosph...	14.198	5.1	ng	179786	5	14.104	703740	20.0
9-Octadecenamid...	14.868	2.9	ng	65779	6	15.616	455030	20.0