LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133878.D
Acq On : 21 Jun 2023 19:01
Operator : CG\JU
Sample : 03289-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-12.0-14.0

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-BF060923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133878.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	10	18	27	rVB	164512	230584	7.84%	0.948%
2	5.110	509	514	526	rBV	364989	470635	16.00%	1.935%
3	5.504	576	581	584	rBV	3075294	2941727	100.00%	12.092%
4	6.504	745	751	753	rBV	2664152	2918397	99.21%	11.996%
5	6.857	808	811	815	rBV	692856	621097	21.11%	2.553%
6	6.916	818	821	831	rVB	35666	36025	1.22%	0.148%
7	7.422	902	907	910	rBV	2068620	1881245	63.95%	7.733%
8	8.139	1025	1029	1032	rBV	878369	724151	24.62%	2.977%
9	9.216	1208	1212	1215	rBV	3585961	2889996	98.24%	11.880%
10	9.486	1252	1258	1264	rBV	82027	73504	2.50%	0.302%
11	9.898	1324	1328	1331	rBV	737663	629984	21.42%	2.590%
12	9.927	1331	1333	1336	rVB	55980	44171	1.50%	0.182%
13	10.445	1418	1421	1424	rBV2	41996	35740	1.21%	0.147%
14	10.610	1445	1449	1453	rBV	126820	112970	3.84%	0.464%
15	10.686	1458	1462	1466	rBV	1674580	1597986	54.32%	6.569%
16	11.386	1578	1581	1584	rBV	633813	638310	21.70%	2.624%
17	11.416	1584	1586	1589	rVV	450592	356882	12.13%	1.467%
18	11.463	1590	1594	1597	rVB	95913	87260	2.97%	0.359%
19	11.621	1615	1621	1627	rBV2	49617	67489	2.29%	0.277%
20	11.892	1664	1667	1669	rBV	74614	65746	2.23%	0.270%
21	11.921	1669	1672	1676	rVV2	193976	208901	7.10%	0.859%
22	11.968	1676	1680	1683	rVV2	41579	58930	2.00%	0.242%
23	12.004	1683	1686	1689	rVV	130576	143636	4.88%	0.590%
24	12.027	1689	1690	1695	rVB	64971	43085	1.46%	0.177%
25	12.192	1715	1718	1720	rBV	55189	44819	1.52%	0.184%
26	12.215	1720	1722	1728	rVB2	51956	47692	1.62%	0.196%
27	12.445	1758	1761	1764	rBV	59338	72728	2.47%	0.299%
28	12.533	1773	1776	1780	rBV3	72978	80218	2.73%	0.330%
29	12.610	1785	1789	1793	rBV	818221	701203	23.84%	2.882%
30	12.839	1822	1828	1834	rBV	693345	767621	26.09%	3.155%
31	12.892	1834	1837	1841	rVB2	33242	42801	1.45%	0.176%
32	12.986	1849	1853	1857	rVV	2767396	2609590	88.71%	10.727%
33	13.057	1861	1865	1870	rBV3	54488	91100	3.10%	0.374%
34	13.145	1877	1880	1882	rBV3	42536	54573	1.86%	0.224%
35	13.168	1882	1884	1888	rVB	82602	86103	2.93%	0.354%
36	13.239	1894	1896	1898	rVB	53300	37639	1.28%	0.155%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
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Acq On : 21 Jun 2023 19:01
Operator : CG\JU
Sample : 03289-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-05-12.0-14.0

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-BF060923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.274	1898	1902	1905	rBV2	81304	80915	2.75%	0.333%
38	13.368	1915	1918	1921	rBV	48825	42232	1.44%	0.174%
39	13.398	1921	1923	1927	rVV	48295	46601	1.58%	0.192%
40	13.680	1969	1971	1977	rVB	67482	74913	2.55%	0.308%
41	13.792	1987	1990	1994	rBV3	57724	72125	2.45%	0.296%
42	13.845	1997	1999	2004	rVV2	38078	53164	1.81%	0.219%
43	13.892	2004	2007	2016	rVB2	106768	157728	5.36%	0.648%
44	14.051	2028	2034	2036	rBV2	707136	929414	31.59%	3.820%
45	14.074	2036	2038	2041	rVB	303163	237753	8.08%	0.977%
46	14.151	2049	2051	2054	rVB2	45159	41752	1.42%	0.172%
47	14.439	2098	2100	2103	rVB	65883	49889	1.70%	0.205%
48	15.109	2210	2214	2217	rBV	192648	281755	9.58%	1.158%
49	15.427	2264	2268	2275	rVB	109545	150335	5.11%	0.618%
50	15.492	2275	2279	2285	rVB	152271	197045	6.70%	0.810%
51	15.556	2285	2290	2294	rBV	306714	397166	13.50%	1.633%

Sum of corrected areas: 24327325

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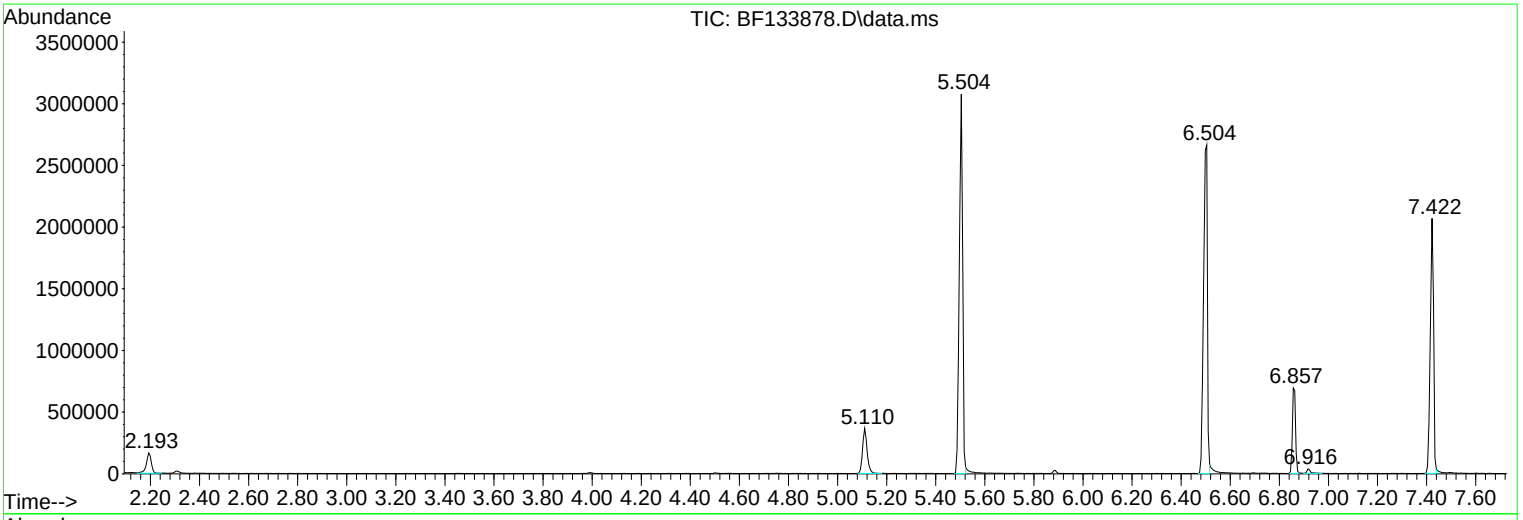
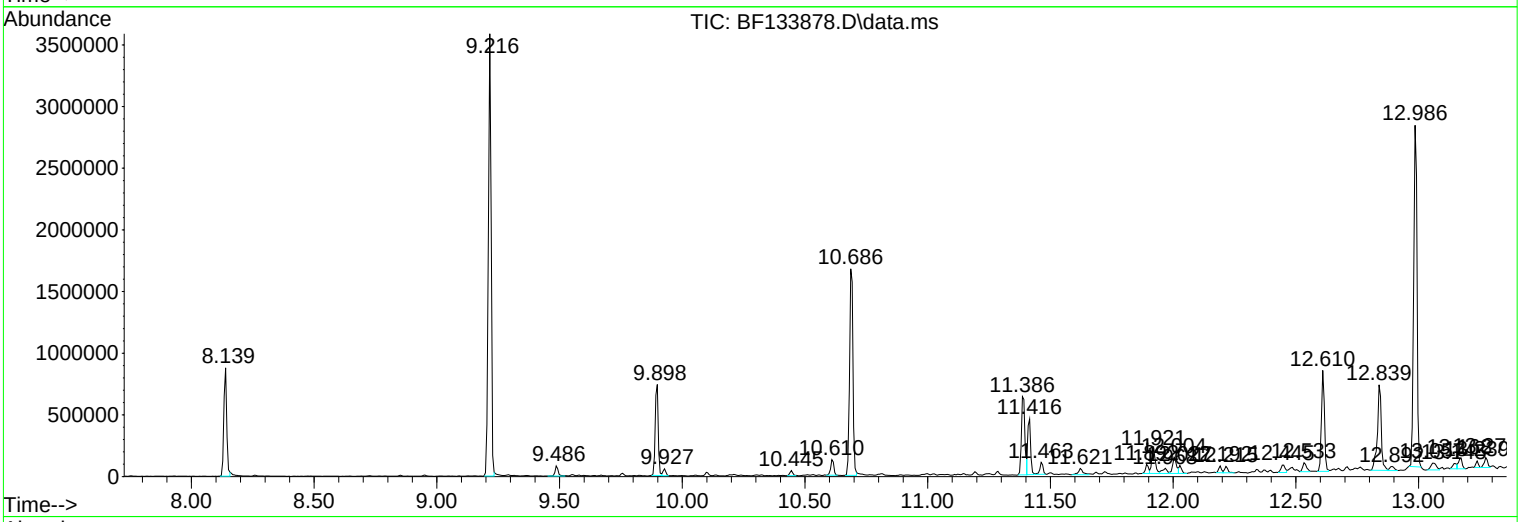
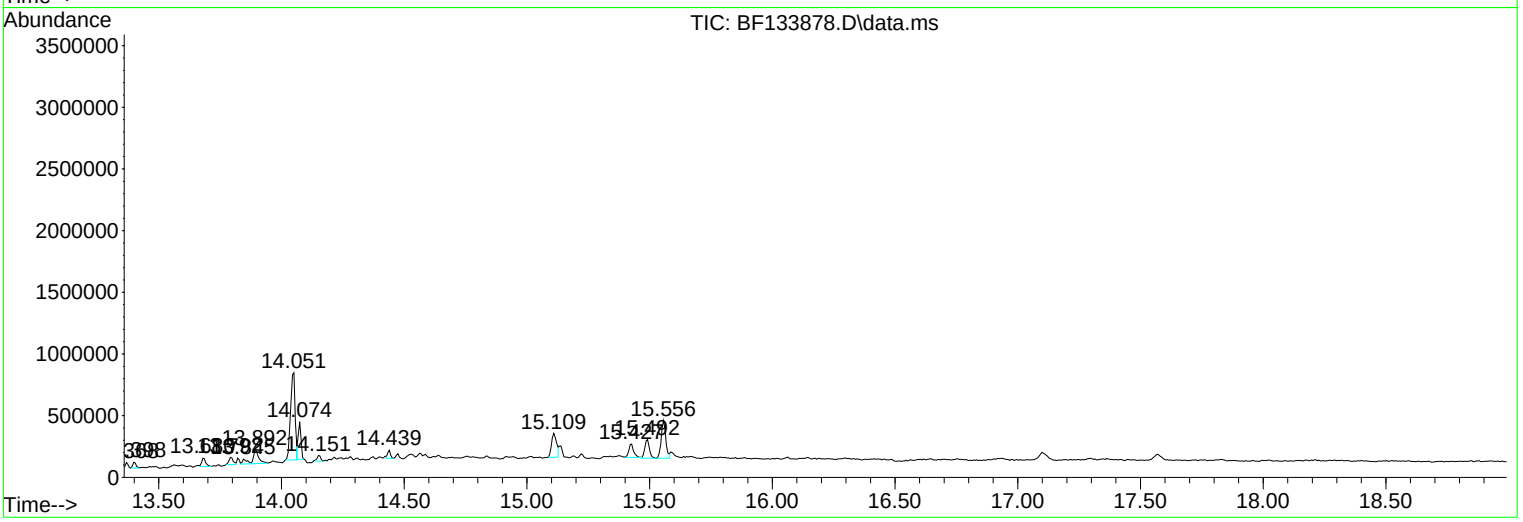
Instrument :
BNA_F
ClientSampleId :
SB-05-12.0-14.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

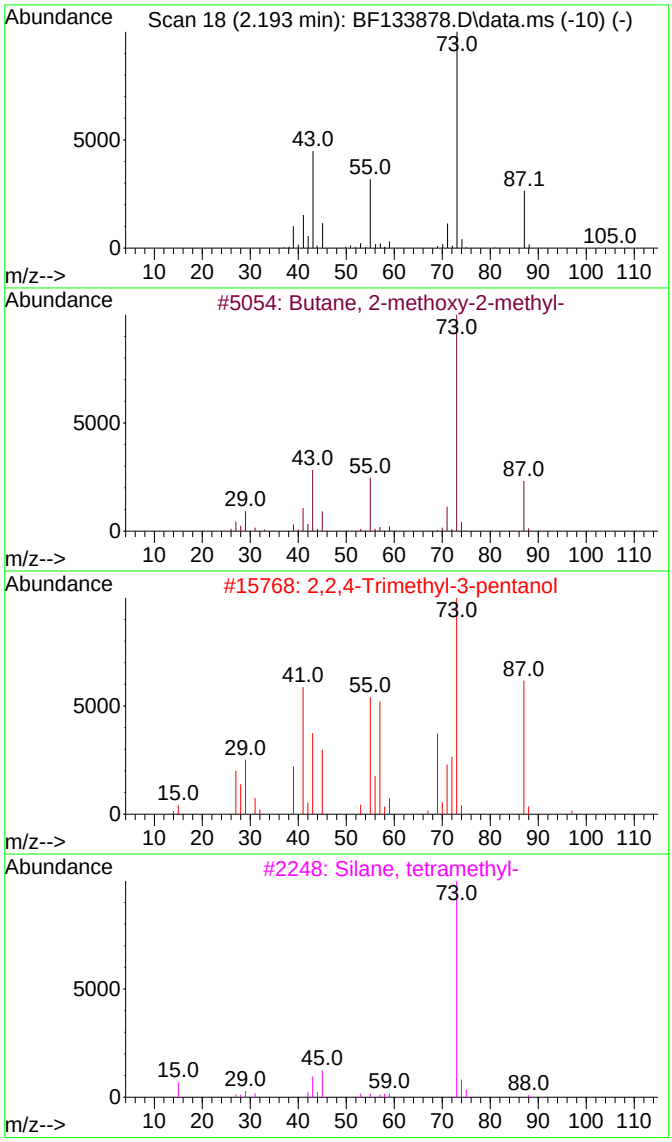
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

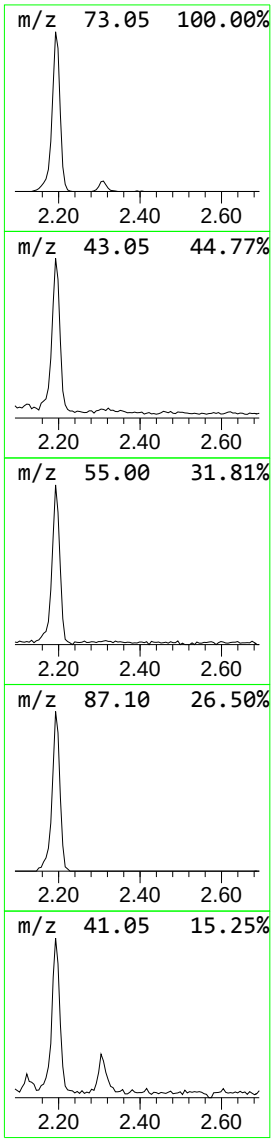
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	7.43 ng	230584	1,4-Dichlorobenzene-d4	6.863

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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Operator : CG\JU
Sample : 03289-13
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ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-12.0-14.0

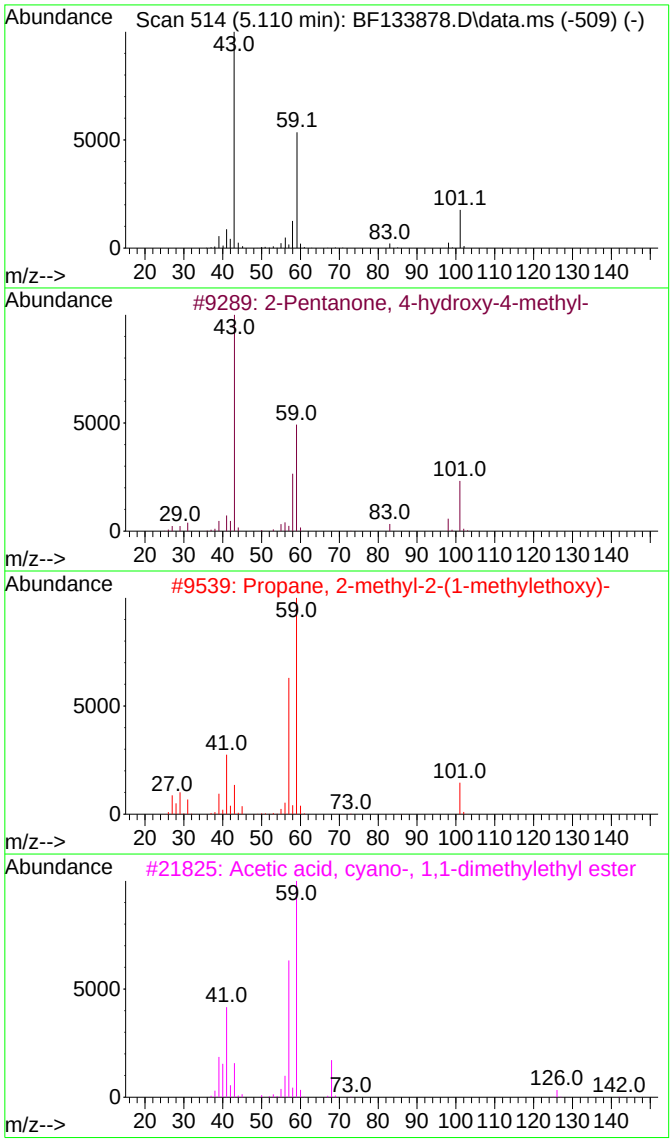
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

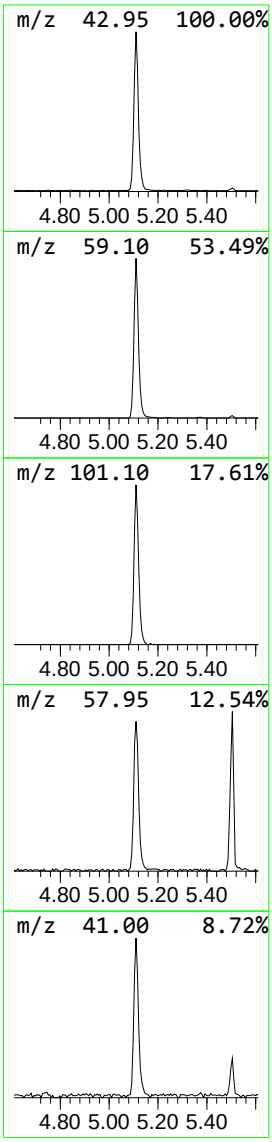
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	15.15 ng	470635	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
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Sample : 03289-13
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ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-12.0-14.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

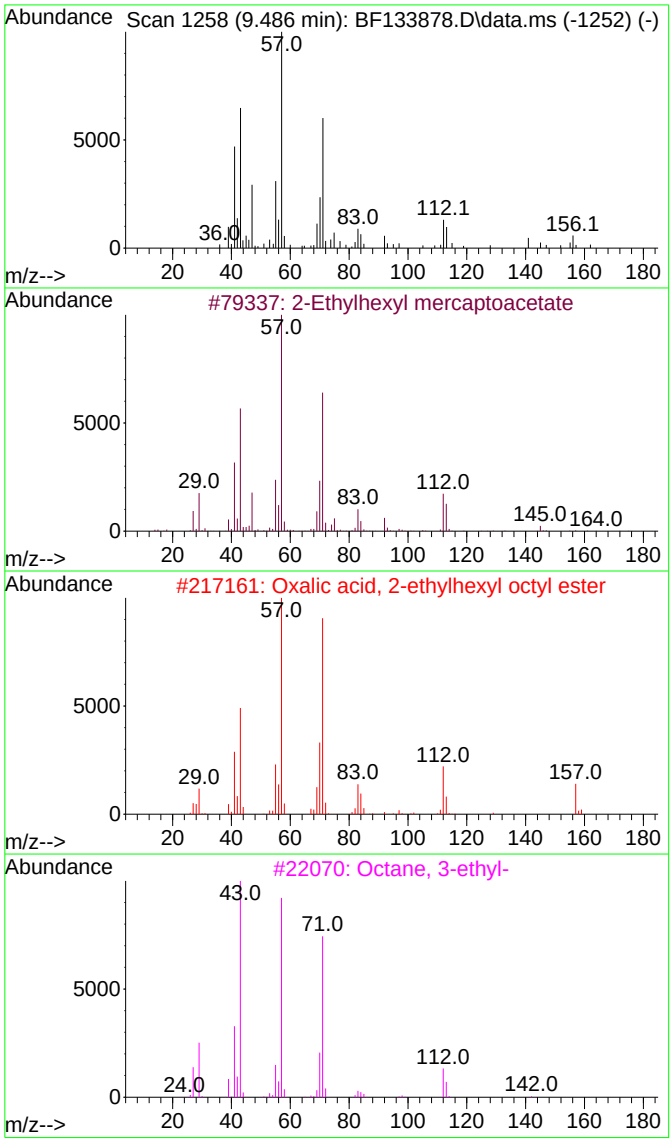
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

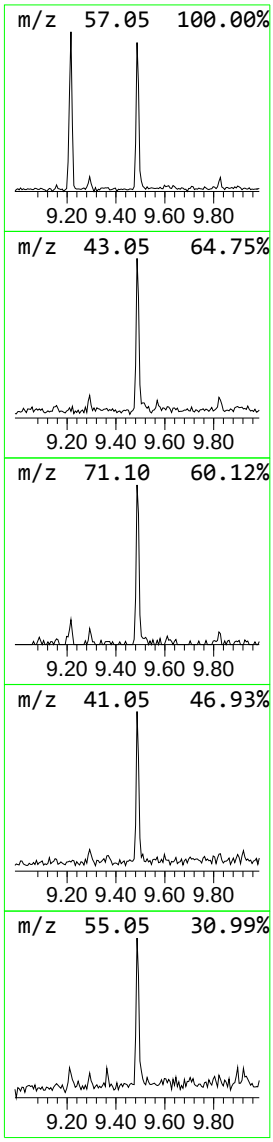
****

Peak Number 3 2-Ethylhexyl mercaptoacetate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.486	2.33 ng	73504	Acenaphthene-d10	9.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethylhexyl mercaptoacetate	204	C10H20O2S	007659-86-1	74
2	Oxalic acid, 2-ethylhexyl octyl ...	314	C18H34O4	1000309-39-1	52
3	Octane, 3-ethyl-	142	C10H22	005881-17-4	50
4	Oxalic acid, 2-ethylhexyl isobut...	258	C14H26O4	1010309-38-5	50
5	Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1010309-19-2	47





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Data File : BF133878.D
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Instrument :
BNA_F
ClientSampleId :
SB-05-12.0-14.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

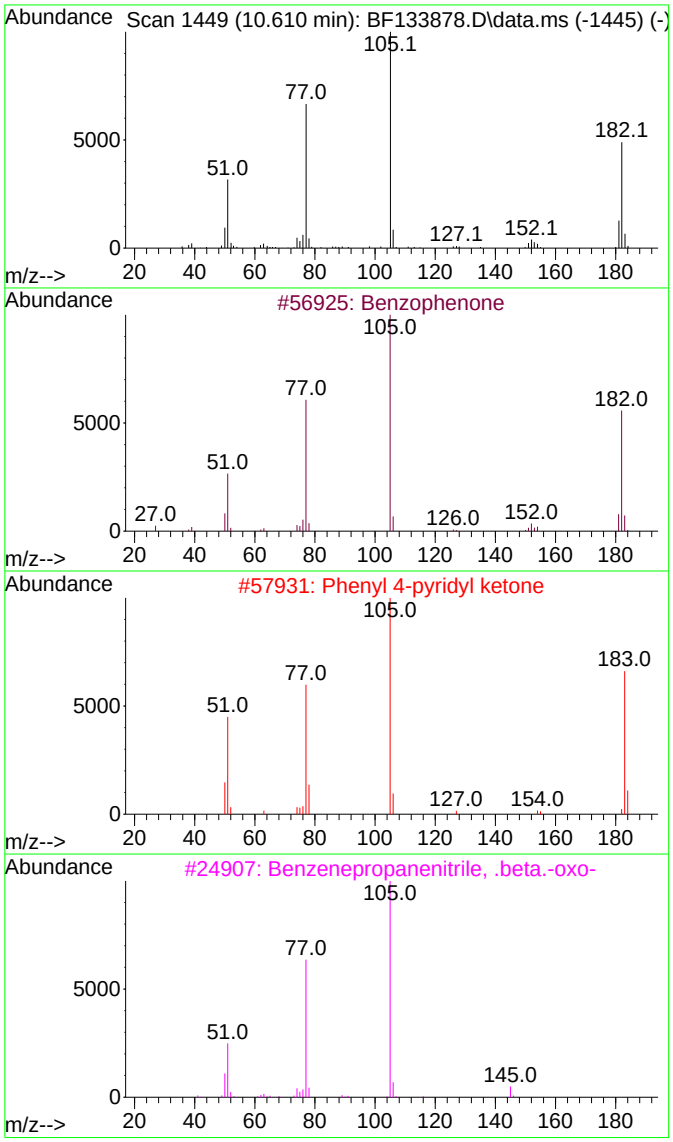
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

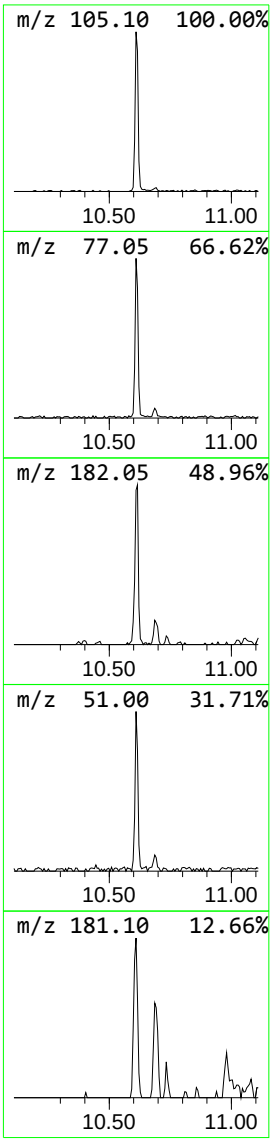
****

Peak Number 4 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.610	3.59 ng	112970	Acenaphthene-d10	9.898

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	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	49
4	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
5	Benzilic acid	228	C14H12O3	000076-93-7	47





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ClientSampleId :
SB-05-12.0-14.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

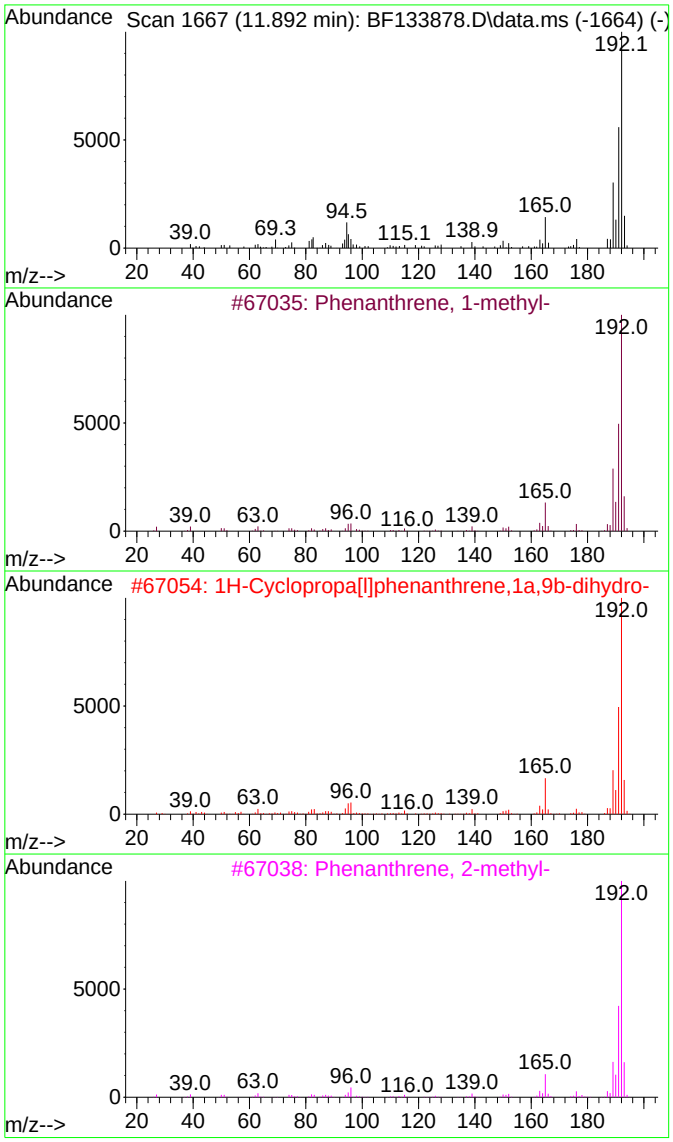
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

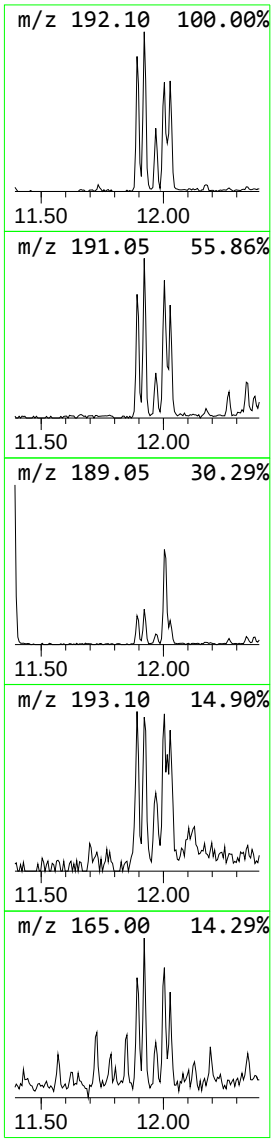
****

Peak Number 6 Phenanthrene, 1-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	2.06 ng	65746	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
2	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	96
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	94
5	1H-Indene, 1-phenyl-	192	C15H12	001961-96-2	93





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BNA_F
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SB-05-12.0-14.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

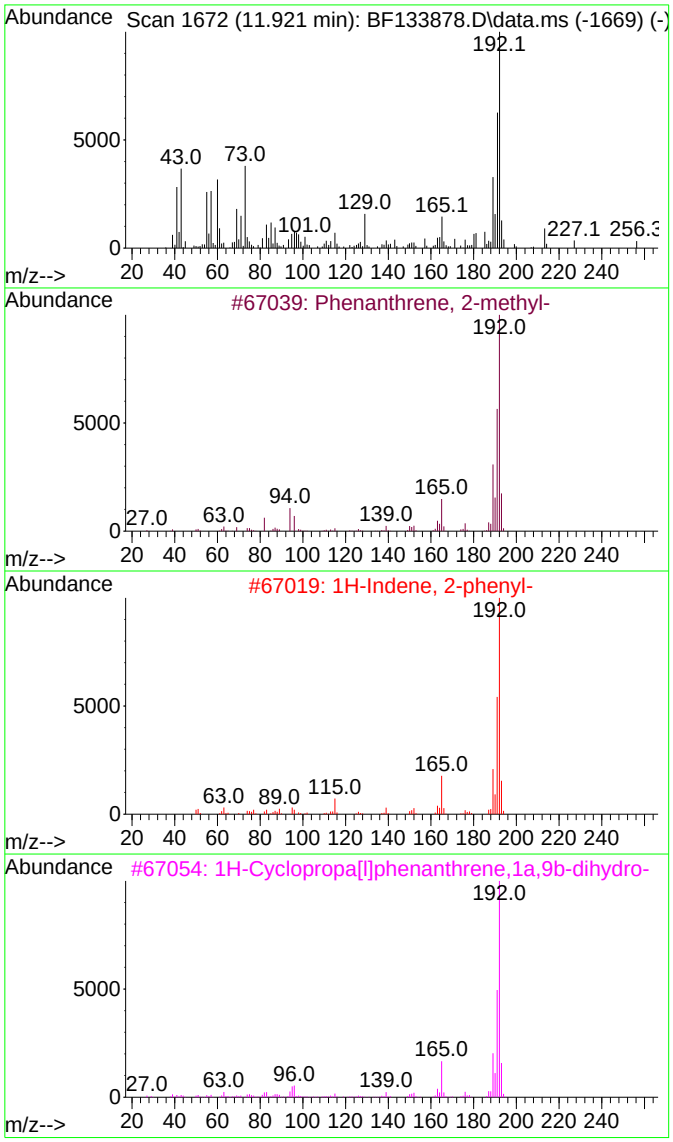
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

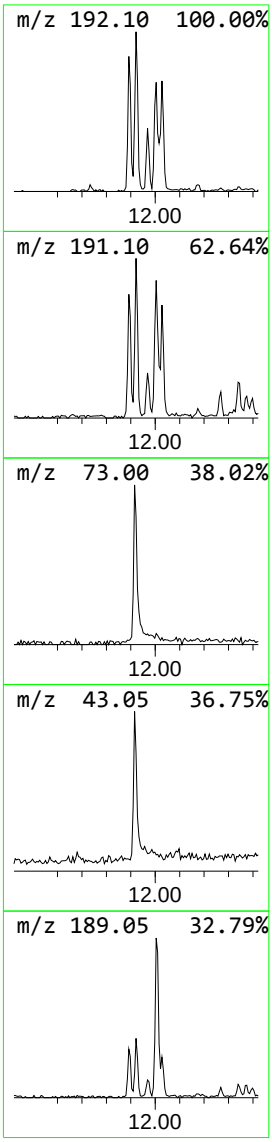
****

Peak Number 7 Phenanthrene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.921	6.55 ng	208901	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93
2	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	93
3	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	92
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	91
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	90





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ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-12.0-14.0

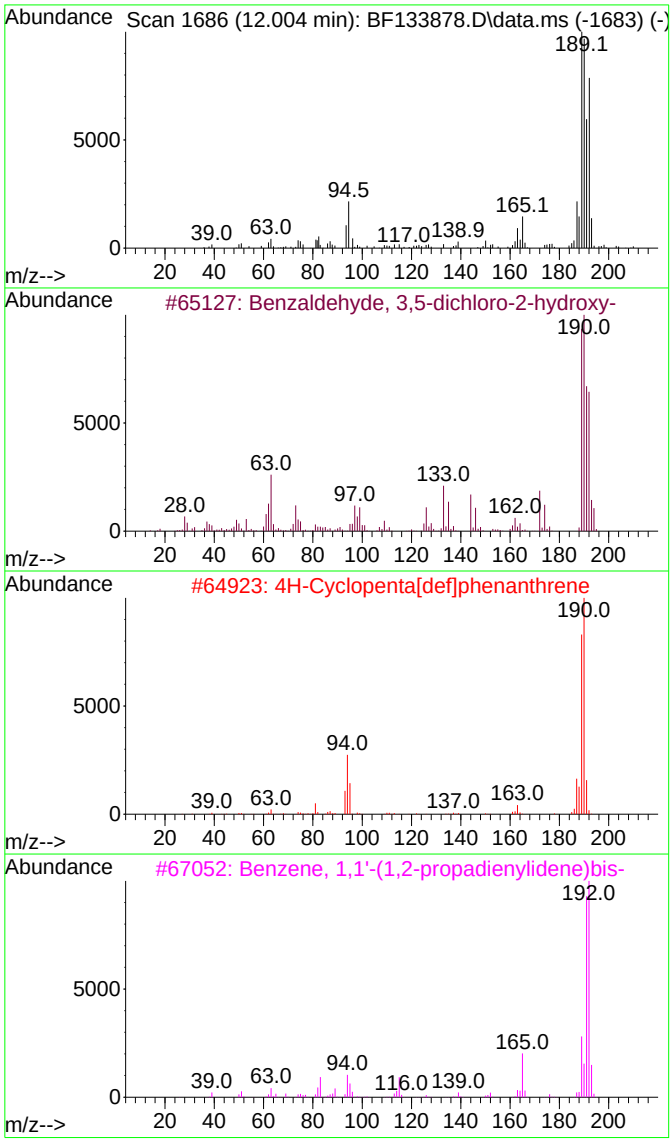
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

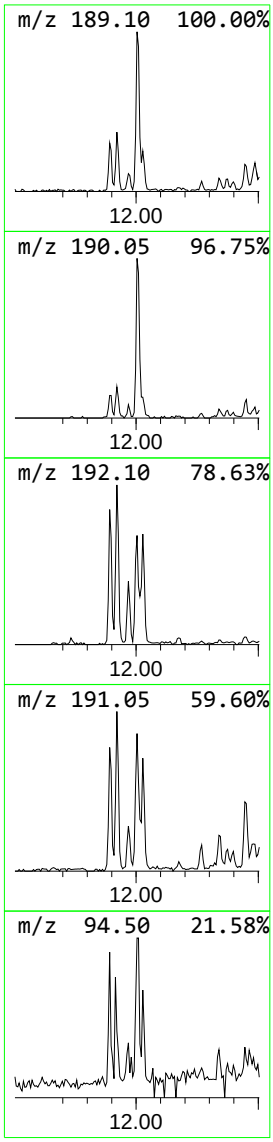
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzaldehyde, 3,5-dichloro-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.004	4.50 ng	143636	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	72
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	49
3	Benzene, 1,1'-(1,2-propadienylid...	192	C15H12	014251-57-1	41
4	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	38
5	Propyne, 1,3-diphenyl-	192	C15H12	004980-70-5	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133878.D
Acq On : 21 Jun 2023 19:01
Operator : CG\JU
Sample : 03289-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-12.0-14.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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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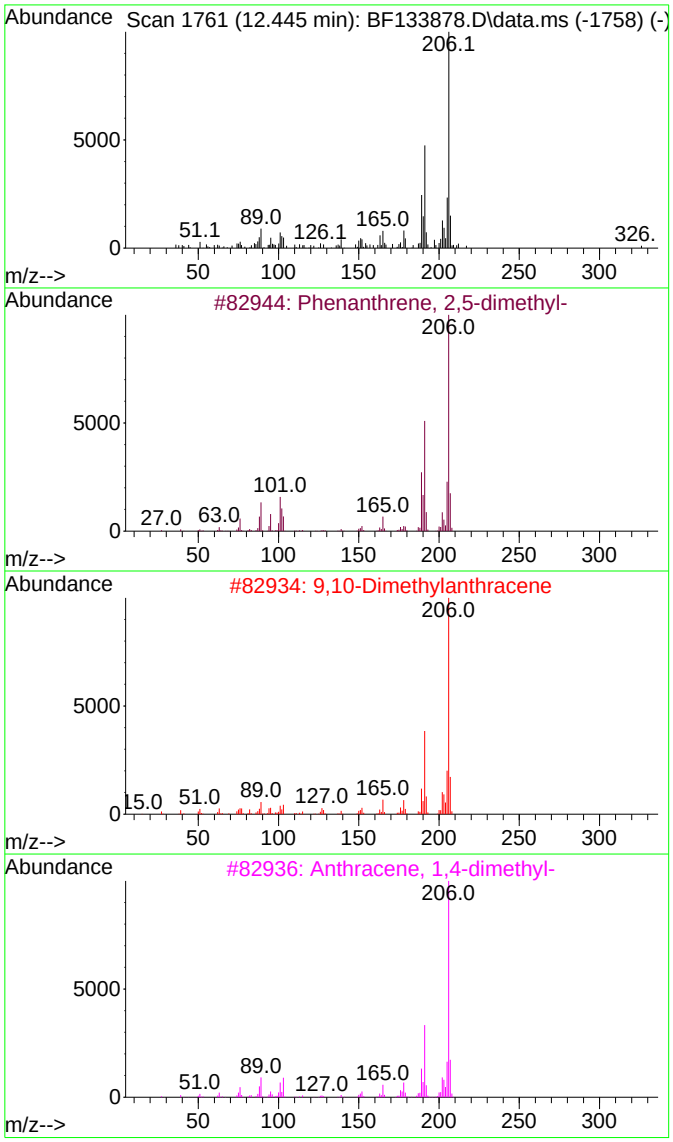
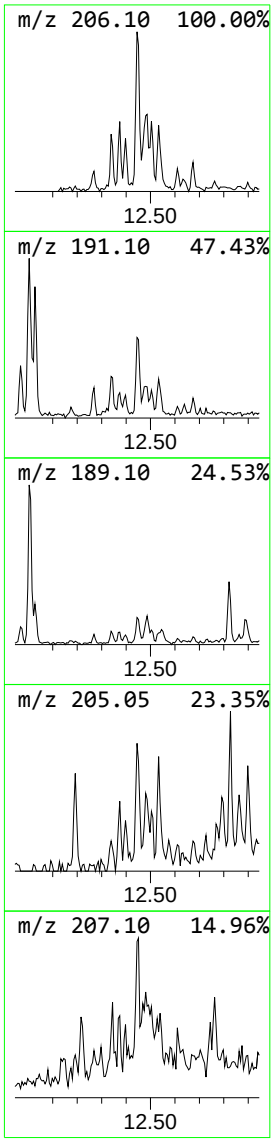
Peak Number 9 Phenanthrene, 2,5-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.445	2.28 ng	72728	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	97
2	9,10-Dimethylanthracene	206	C16H14	000781-43-1	95
3	Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	91
4	3-Methyl-1-phenyl-1H-indene	206	C16H14	022360-63-0	90
5	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	87





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Data File : BF133878.D
Acq On : 21 Jun 2023 19:01
Operator : CG\JU
Sample : 03289-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-12.0-14.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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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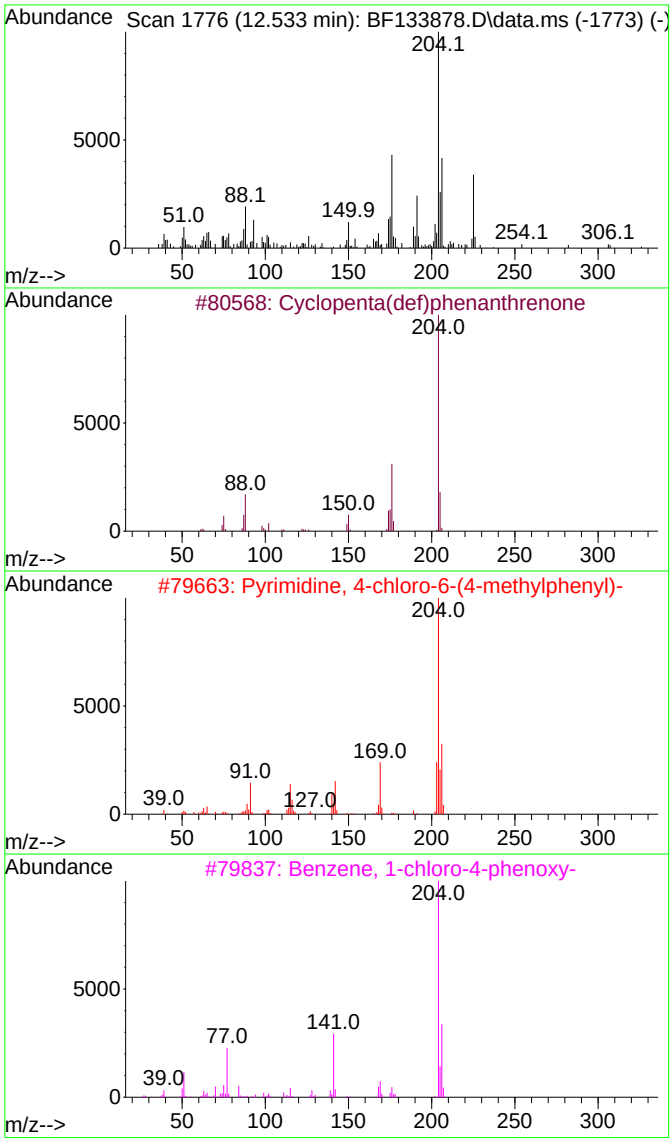
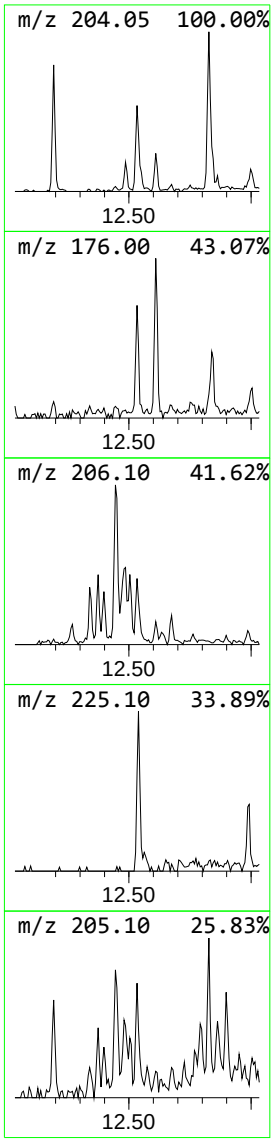
Peak Number 10 Cyclopenta(def)phenanthrenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.533	2.51 ng	80218	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	95
2	Pyrimidine, 4-chloro-6-(4-methyl...	204	C11H9ClN2	1000380-55-8	43
3	Benzene, 1-chloro-4-phenoxy-	204	C12H9ClO	007005-72-3	43
4	3,4-Biphenyldicarbonitrile	204	C14H8N2	004128-63-6	38
5	2-Chloro-4-phenylphenol	204	C12H9ClO	000092-04-6	32





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Operator : CG\JU
Sample : 03289-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-12.0-14.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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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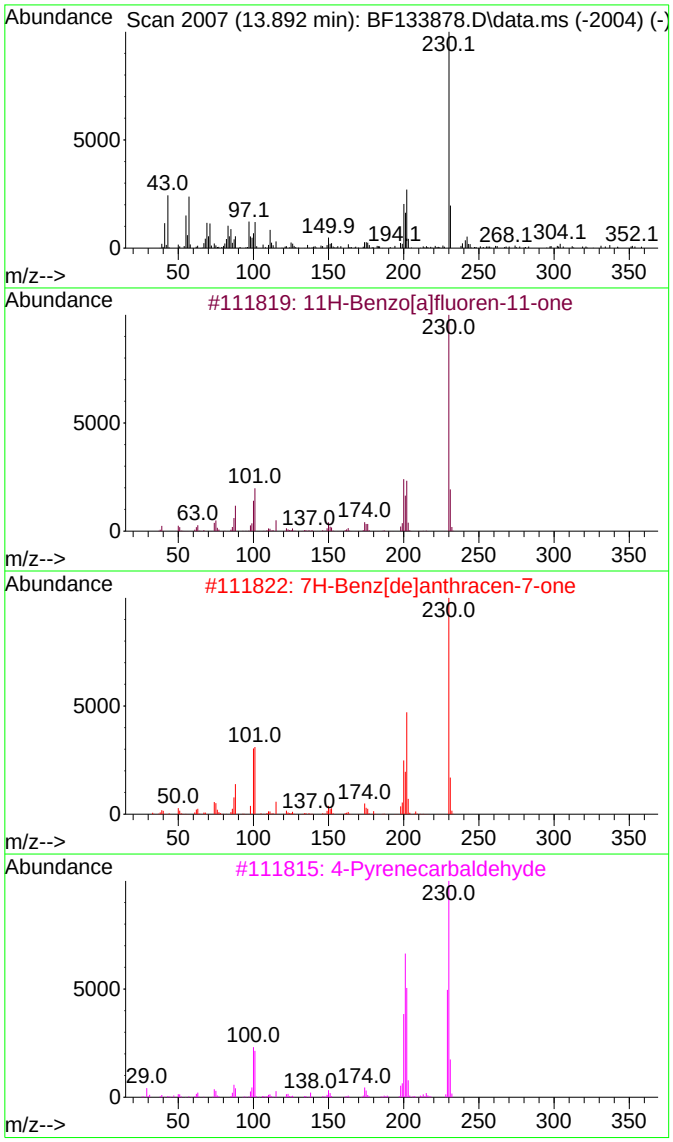
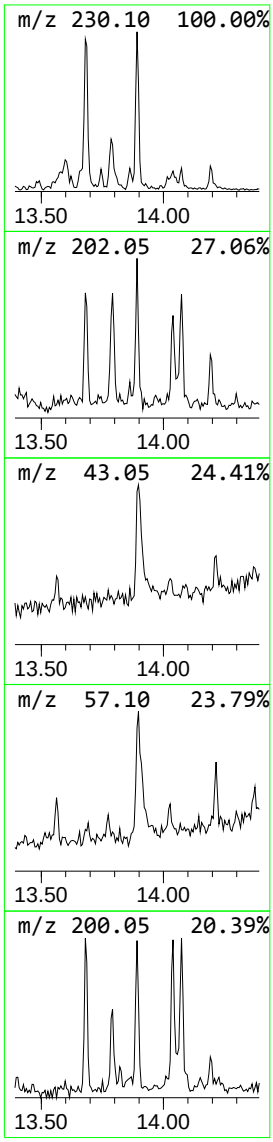
Peak Number 11 11H-Benzo[a]fluoren-11-one Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	3.39 ng	157728	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	93
2	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	87
3	4-Pyrenecarbaldehyde	230	C17H10O	022245-51-8	72
4	6H-Benz[de]anthracen-6-one	230	C17H10O	080252-14-8	59
5	benzonitrile, 2-(3-isoquinolinyl)-	230	C16H10N2	1000401-00-3	59





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Data File : BF133878.D
Acq On : 21 Jun 2023 19:01
Operator : CG\JU
Sample : 03289-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-12.0-14.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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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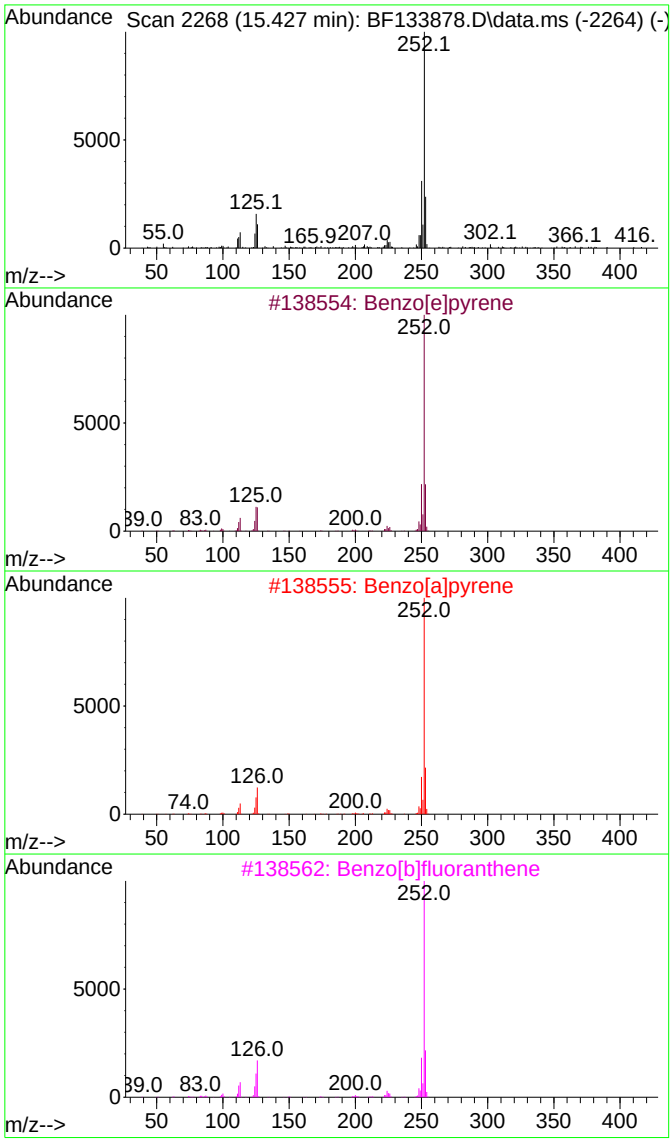
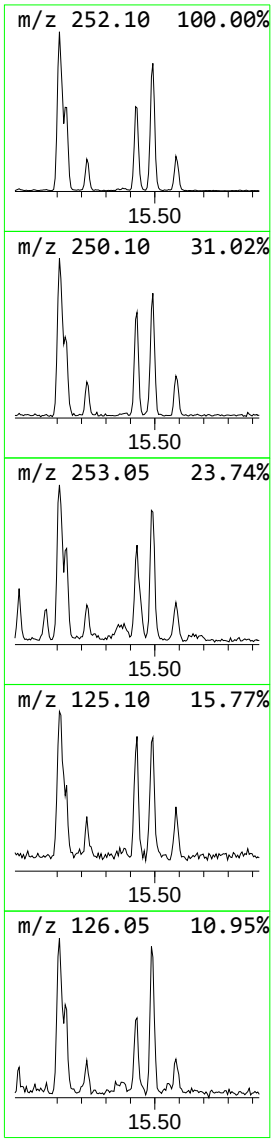
Peak Number 12 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.427	7.57 ng	150335	Perylene-d12	15.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2	Benzo[a]pyrene	252	C20H12	000050-32-8	94
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	90
4	Perylene	252	C20H12	000198-55-0	89
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133878.D
Acq On : 21 Jun 2023 19:01
Operator : CG\JU
Sample : 03289-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-12.0-14.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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	7.4	ng	230584	1	6.863	621097	20.0
2-Pentanone, 4-...	5.110	15.2	ng	470635	1	6.863	621097	20.0
2-Ethylhexyl me...	9.486	2.3	ng	73504	3	9.898	629984	20.0
Benzophenone	10.610	3.6	ng	112970	3	9.898	629984	20.0
Phenanthrene, 1...	11.892	2.1	ng	65746	4	11.386	638310	20.0
Phenanthrene, 2...	11.921	6.5	ng	208901	4	11.386	638310	20.0
Benzaldehyde, 3...	12.004	4.5	ng	143636	4	11.386	638310	20.0
Phenanthrene, 2...	12.445	2.3	ng	72728	4	11.386	638310	20.0
Cyclopenta(def)...	12.533	2.5	ng	80218	4	11.386	638310	20.0
11H-Benzo[a]flu...	13.892	3.4	ng	157728	5	14.051	929414	20.0
Benzo[e]pyrene	15.427	7.6	ng	150335	6	15.556	397166	20.0