LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139193.D
Acq On : 27 Aug 2024 18:23
Operator : RC/JU
Sample : P3739-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-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-BF082724.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139193.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	7	14	21	rVB	1123745	1714444	84.45%	9.301%
2	3.375	213	218	229	rBV	45163	95261	4.69%	0.517%
3	5.099	503	511	520	rVB	68581	102556	5.05%	0.556%
4	5.504	574	580	585	rBV	1115520	1429956	70.44%	7.758%
5	6.510	745	751	756	rBV	1172941	1534516	75.59%	8.325%
6	6.710	780	785	797	rBV	51212	64641	3.18%	0.351%
7	6.893	810	816	821	rVB	405200	506602	24.95%	2.748%
8	7.451	905	911	916	rBV	707325	912130	44.93%	4.949%
9	7.704	950	954	958	rBV	20847	24067	1.19%	0.131%
10	8.169	1028	1033	1042	rBV	504964	647000	31.87%	3.510%
11	8.481	1081	1086	1096	rBV	82975	106283	5.24%	0.577%
12	9.245	1210	1216	1221	rBV	1283811	1550242	76.36%	8.411%
13	9.922	1326	1331	1336	rBV	570109	689878	33.98%	3.743%
14	10.022	1341	1348	1354	rBV	1317347	2030166	100.00%	11.014%
15	10.710	1459	1465	1480	rVB	733348	938942	46.25%	5.094%
16	11.410	1579	1584	1592	rBV2	488119	818812	40.33%	4.442%
17	11.481	1592	1596	1600	rVB	30186	37890	1.87%	0.206%
18	11.633	1616	1622	1631	rBV2	16649	26108	1.29%	0.142%
19	11.933	1664	1673	1678	rBV2	84122	139807	6.89%	0.758%
20	12.022	1684	1688	1697	rVB	35833	65175	3.21%	0.354%
21	12.204	1715	1719	1726	rBV2	16586	36707	1.81%	0.199%
22	12.457	1757	1762	1766	rBV	20412	30735	1.51%	0.167%
23	12.504	1766	1770	1774	rVV6	17578	33123	1.63%	0.180%
24	12.622	1782	1790	1794	rBV	265069	348694	17.18%	1.892%
25	12.845	1822	1828	1834	rBV	255353	374078	18.43%	2.029%
26	12.992	1844	1853	1860	rVB	979679	1241929	61.17%	6.738%
27	13.063	1860	1865	1873	rBV3	22125	45790	2.26%	0.248%
28	13.175	1873	1884	1887	rBV2	30070	65039	3.20%	0.353%
29	13.239	1887	1895	1898	rBV2	20503	36482	1.80%	0.198%
30	13.280	1898	1902	1905	rVB2	24887	31697	1.56%	0.172%
31	13.569	1947	1951	1960	rBV7	13961	25157	1.24%	0.136%
32	13.680	1965	1970	1976	rVB	22283	34626	1.71%	0.188%
33	13.792	1983	1989	1992	rBV2	26019	46949	2.31%	0.255%
34	13.892	2002	2006	2013	rVB4	68718	112833	5.56%	0.612%
35	14.045	2024	2032	2043	rBV2	498806	962228	47.40%	5.220%
36	14.151	2044	2050	2053	rBV2	18293	27320	1.35%	0.148%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
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Acq On : 27 Aug 2024 18:23
Operator : RC/JU
Sample : P3739-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-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-BF082724.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.222	2058	2062	2066	rVV5	14678	26163	1.29%	0.142%
38	14.427	2093	2097	2101	rBV	25885	31947	1.57%	0.173%
39	14.521	2108	2113	2116	rBV3	28932	44240	2.18%	0.240%
40	14.816	2158	2163	2174	rVV4	43842	95314	4.69%	0.517%
41	14.927	2175	2182	2189	rVB3	10830	29616	1.46%	0.161%
42	15.086	2203	2209	2220	rBV	140411	322943	15.91%	1.752%
43	15.192	2220	2227	2233	rVB3	25371	52416	2.58%	0.284%
44	15.392	2256	2261	2266	rVB	75466	118387	5.83%	0.642%
45	15.451	2266	2271	2277	rVV	106323	159462	7.85%	0.865%
46	15.516	2277	2282	2296	rVB	276861	481177	23.70%	2.611%
47	16.821	2496	2504	2511	rBV5	9456	24273	1.20%	0.132%
48	16.986	2525	2532	2541	rVB2	38643	85875	4.23%	0.466%
49	17.427	2601	2607	2620	rVB	32011	72409	3.57%	0.393%

Sum of corrected areas: 18432085

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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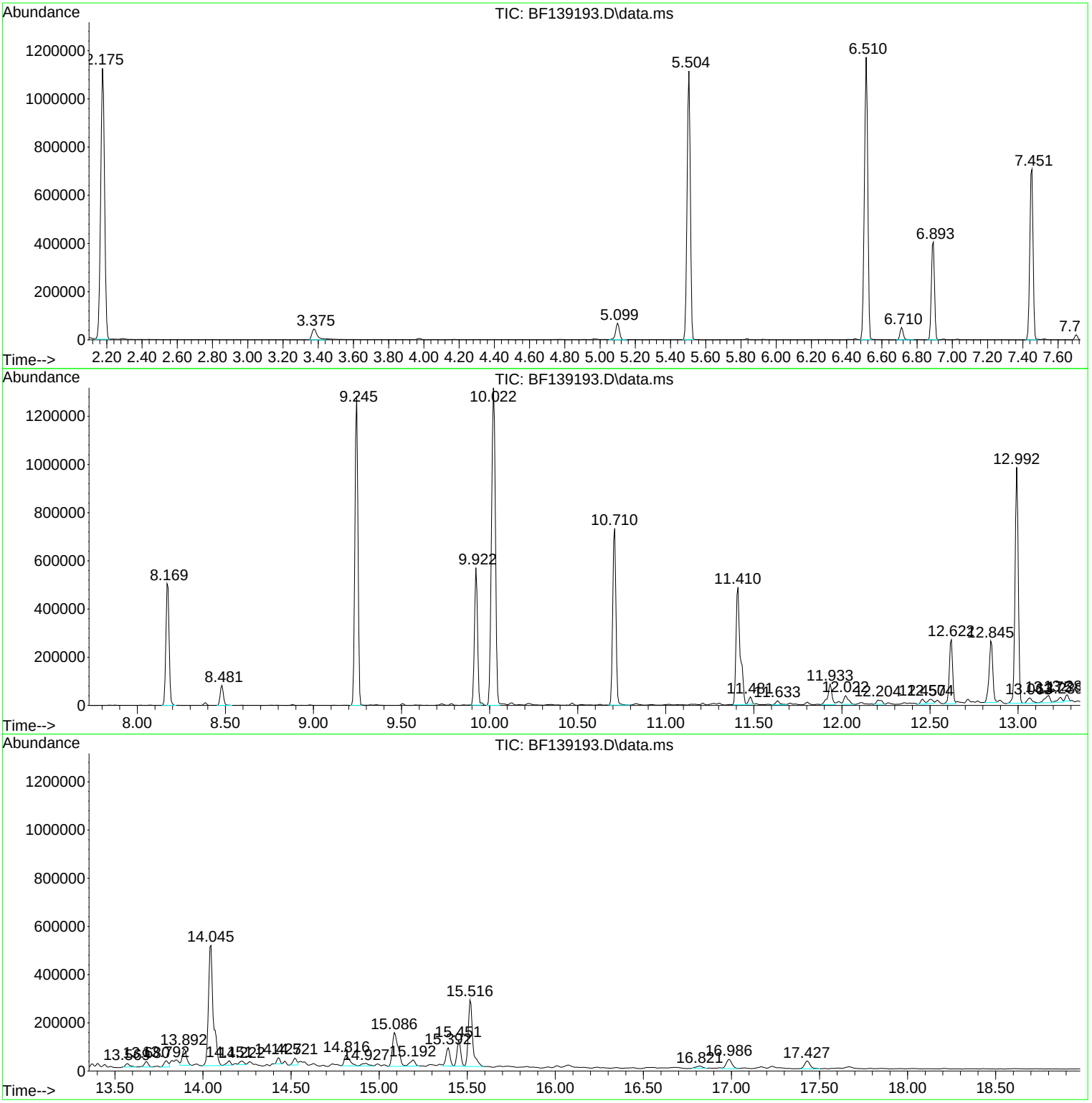
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139193.D
Acq On : 27 Aug 2024 18:23
Operator : RC/JU
Sample : P3739-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

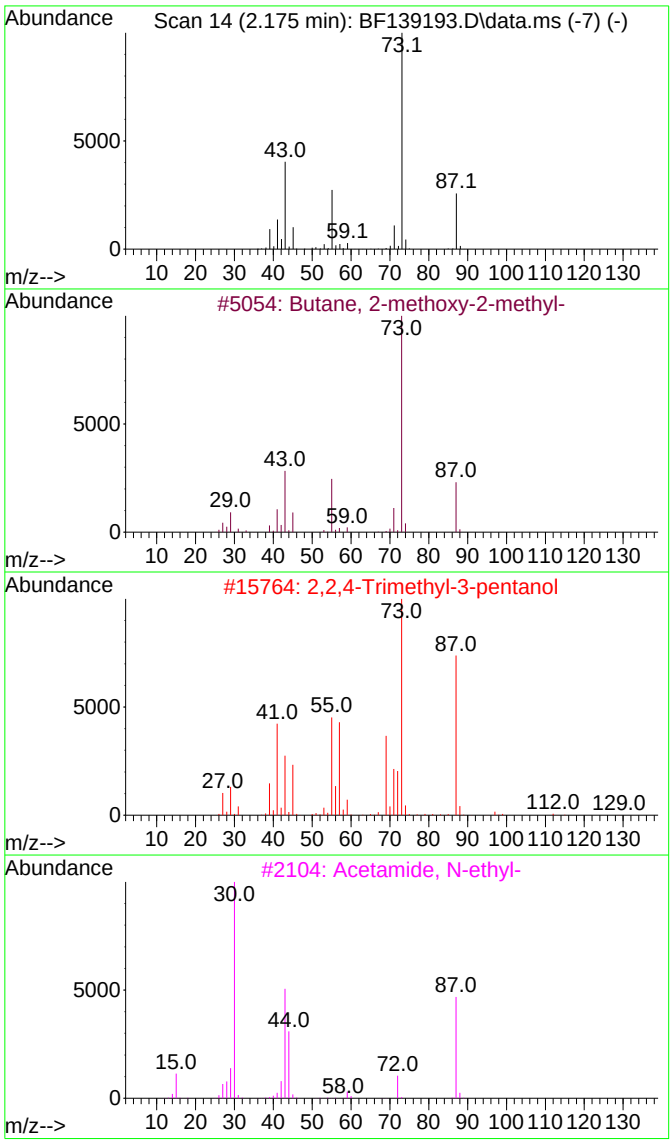
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

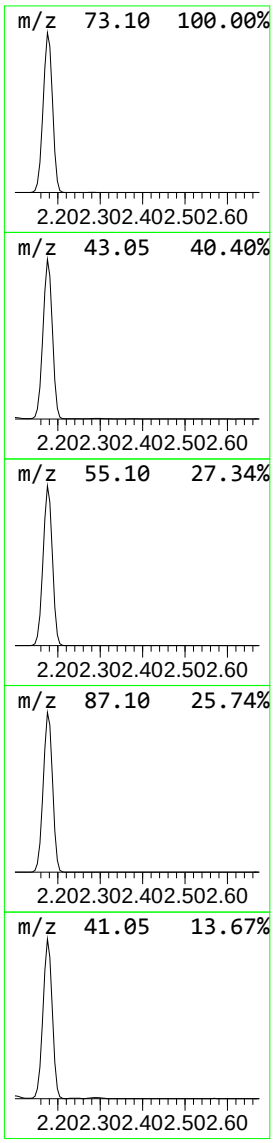
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	67.68 ng	1714440	1,4-Dichlorobenzene-d4	6.893

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	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139193.D
Acq On : 27 Aug 2024 18:23
Operator : RC/JU
Sample : P3739-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

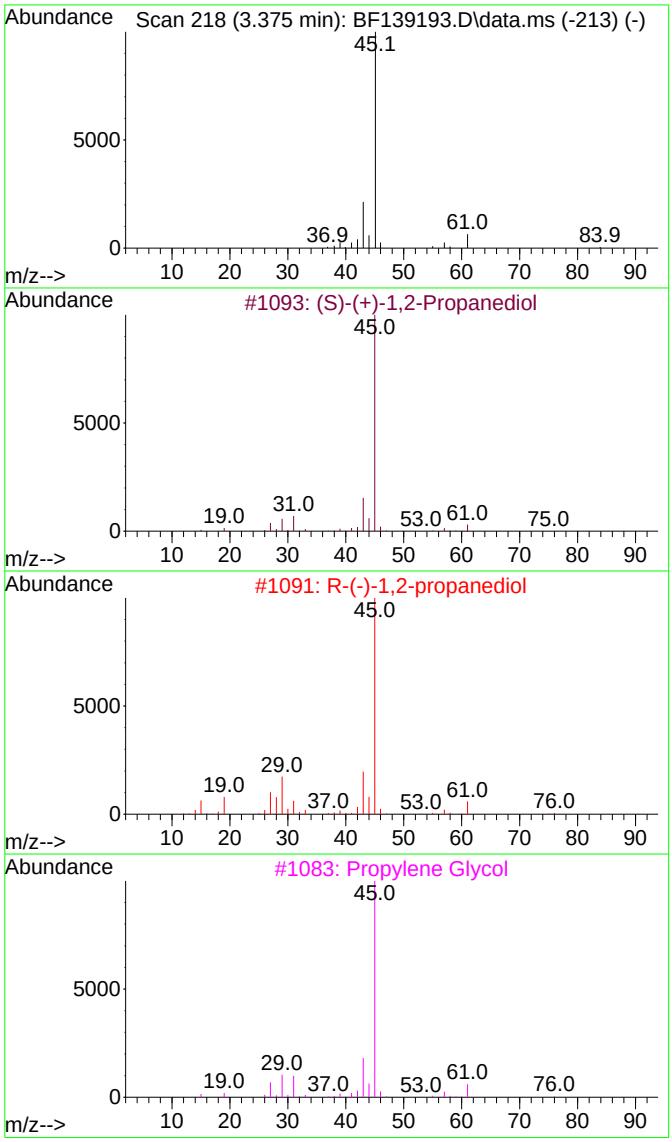
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

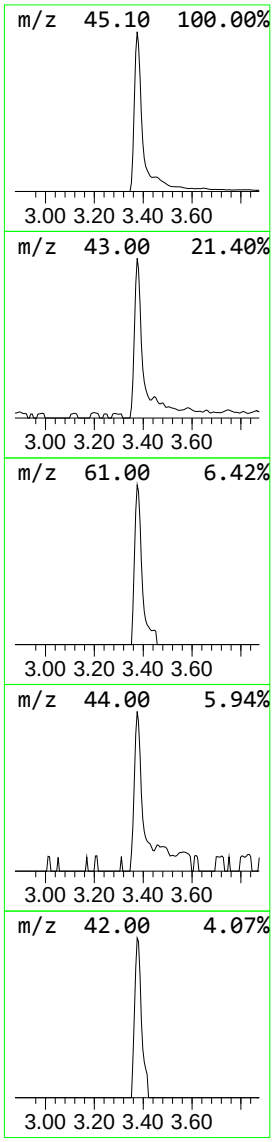
****

Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.375	3.76 ng	95261	1,4-Dichlorobenzene-d4	6.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
3	Propylene Glycol	76	C3H8O2	000057-55-6	9
4	2-Heptanol, (S)-	116	C7H16O	006033-23-4	9
5	2-Heptanol	116	C7H16O	000543-49-7	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139193.D
Acq On : 27 Aug 2024 18:23
Operator : RC/JU
Sample : P3739-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

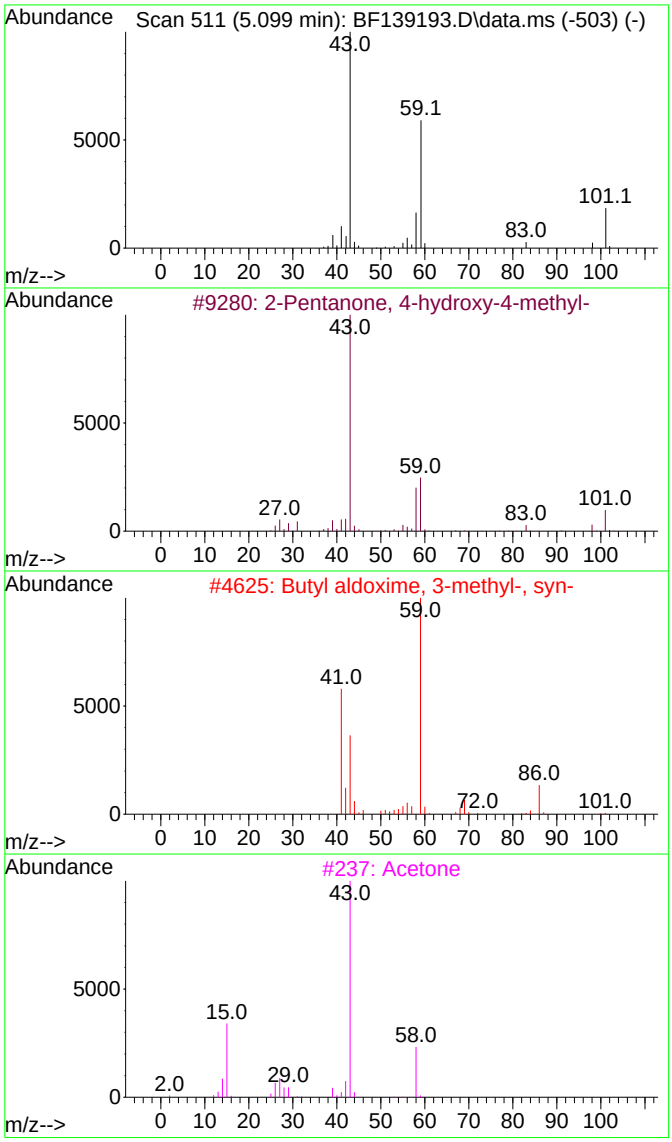
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

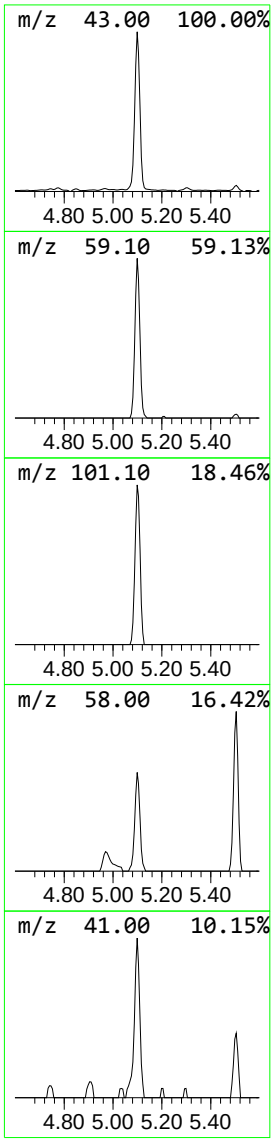
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.099	4.05 ng	102556	1,4-Dichlorobenzene-d4	6.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
3	Acetone	58	C3H6O	000067-64-1	12
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
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Operator : RC/JU
Sample : P3739-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

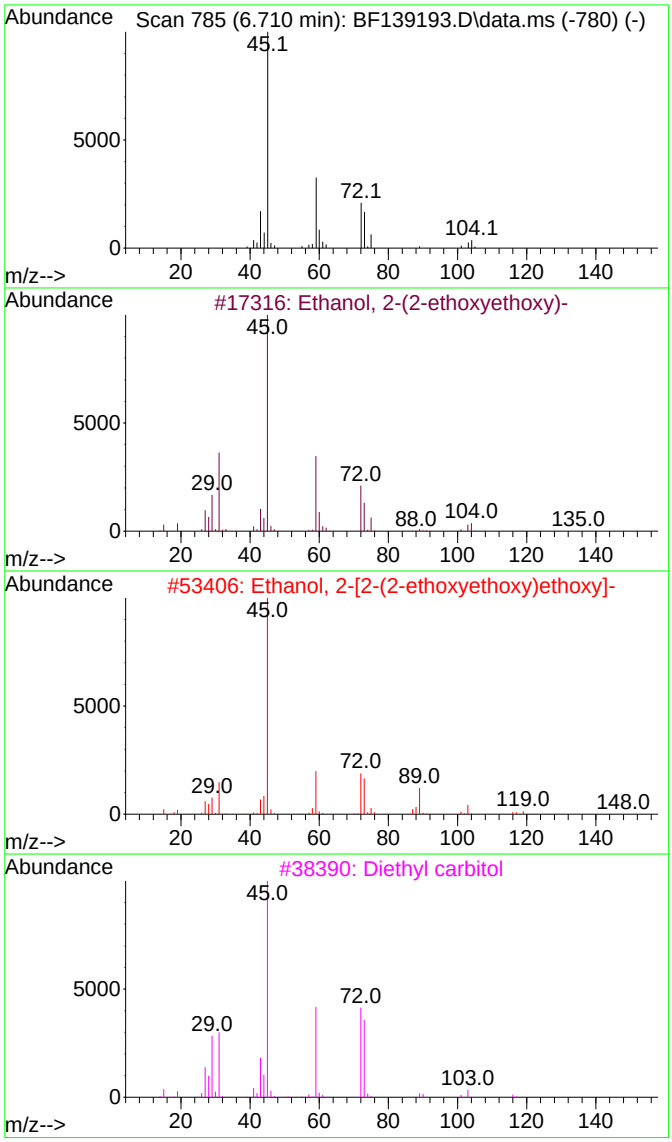
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

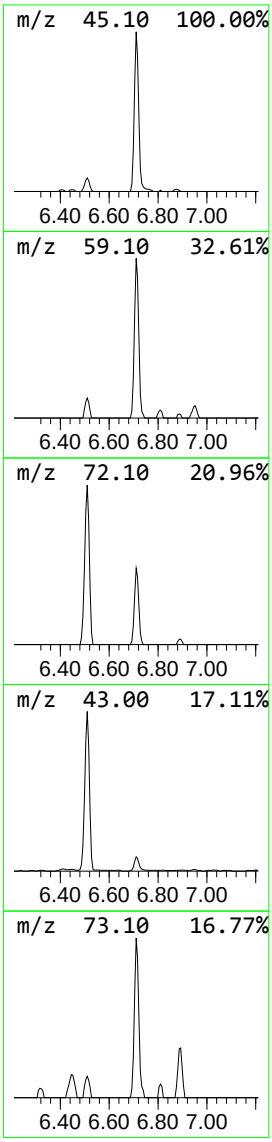
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.710	2.55 ng	64641	1,4-Dichlorobenzene-d4	6.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	78
3	Diethyl carbitol	162	C8H18O3	000112-36-7	78
4	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
5	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139193.D
Acq On : 27 Aug 2024 18:23
Operator : RC/JU
Sample : P3739-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

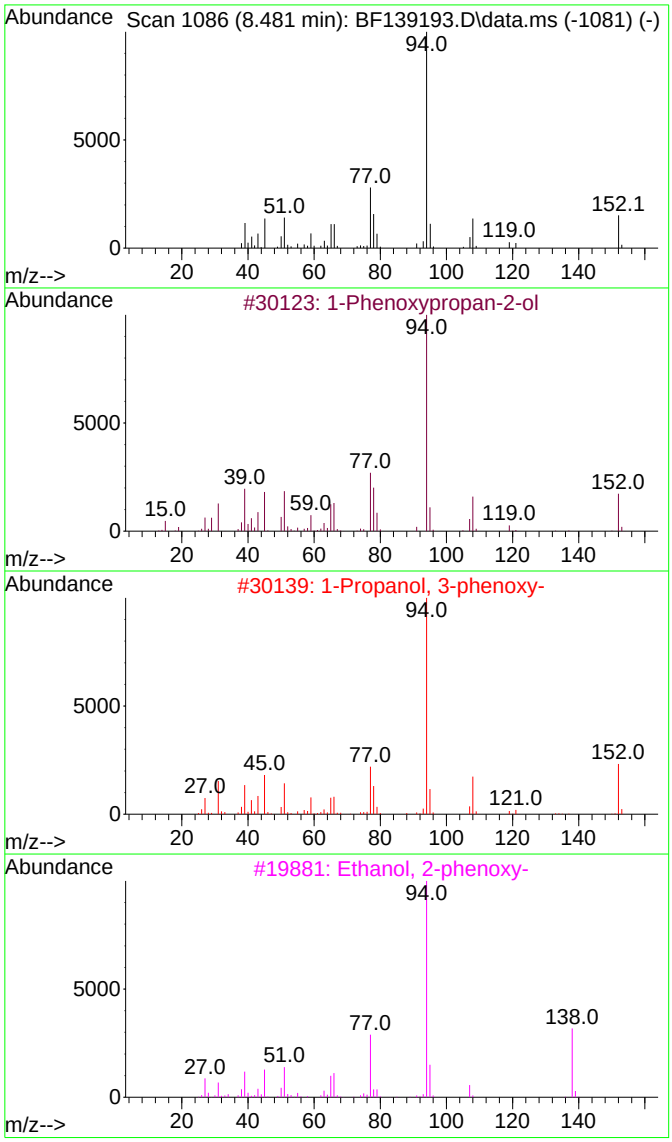
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

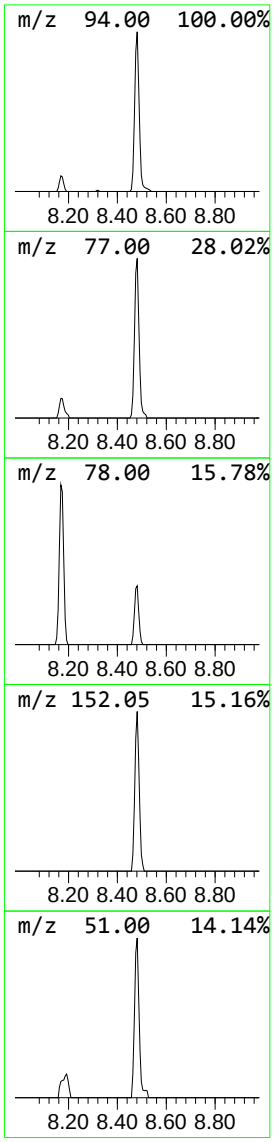
****

Peak Number 5 1-Phenoxypropan-2-ol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.481	3.29 ng	106283	Naphthalene-d8	8.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	3-(.alpha.-Hydroxyethyl)-aniline	137	C8H11NO	002454-37-7	59
5	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59





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ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

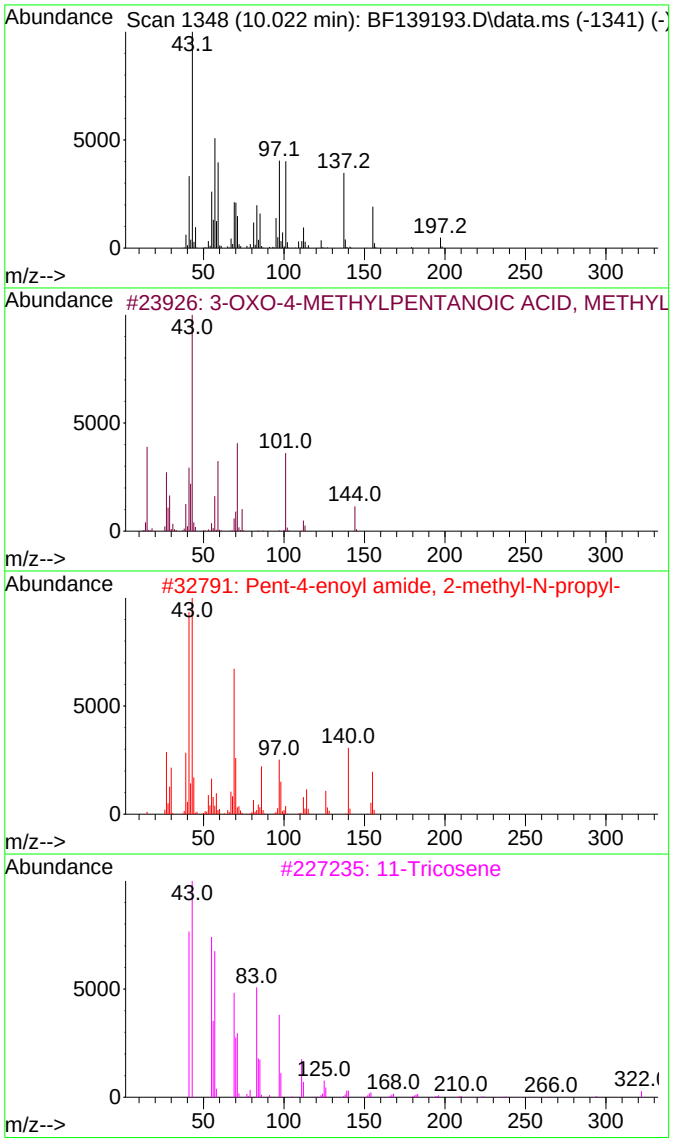
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

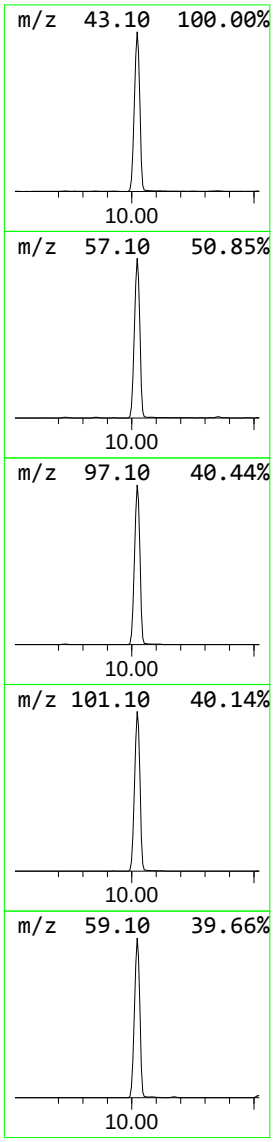
****

Peak Number 6 unknown10.022 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.022	58.86 ng	2030170	Acenaphthene-d10	9.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-OXO-4-METHYLPENTANOIC ACID, ME...	144	C7H12O3	042558-54-3	16
2	Pent-4-enoyl amide, 2-methyl-N-p...	155	C9H17NO	1000420-35-2	14
3	11-Tricosene	322	C23H46	052078-56-5	12
4	2-Pentanol, 2-methyl-, acetate	144	C8H16O2	034859-98-8	10
5	2,4,4-Trimethyl-1-pentanol, chlo...	242	C10H17ClF2O2	1000447-27-2	10





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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

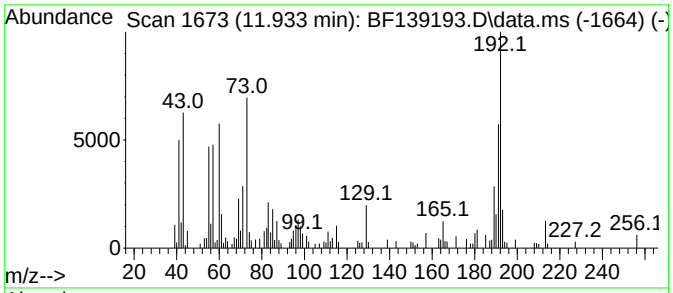
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

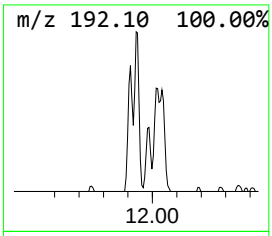
****

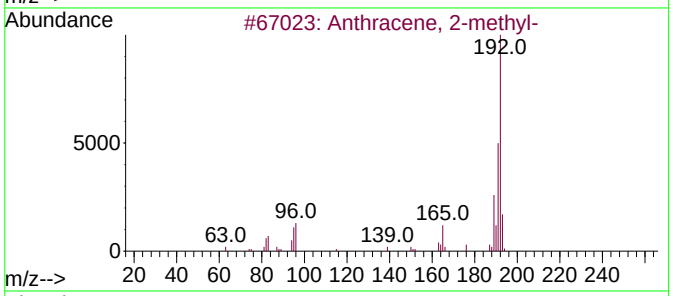
Peak Number 7 Anthracene, 2-methyl- Concentration Rank 7

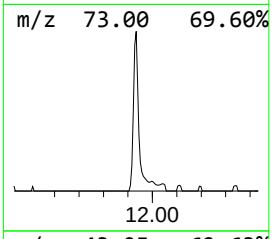
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	3.41 ng	139807	Phenanthrene-d10	11.410

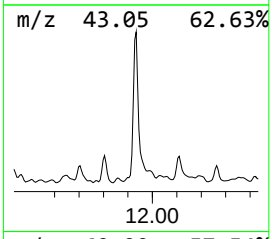
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	91
3	Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	91
4	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	90
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	90

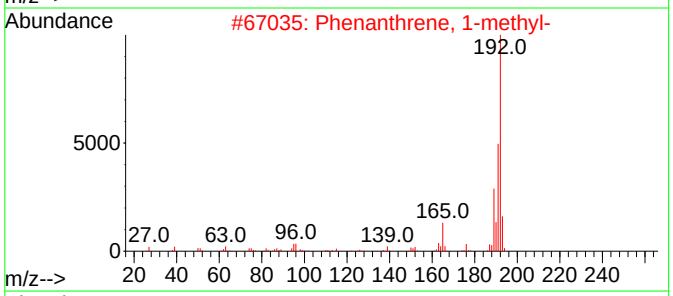


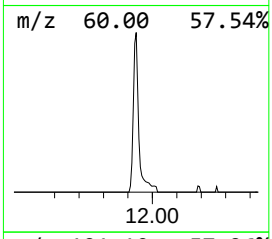


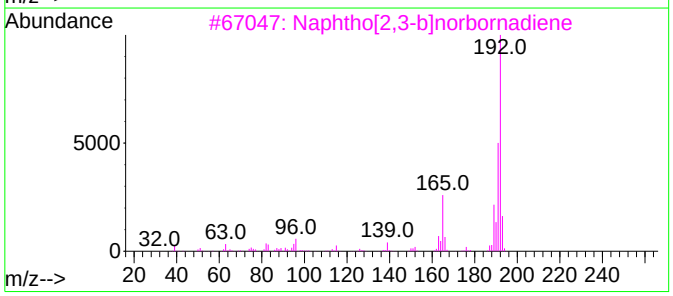


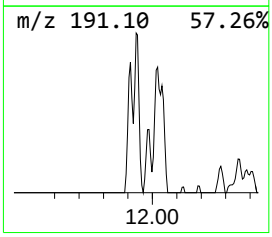












Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139193.D
Acq On : 27 Aug 2024 18:23
Operator : RC/JU
Sample : P3739-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

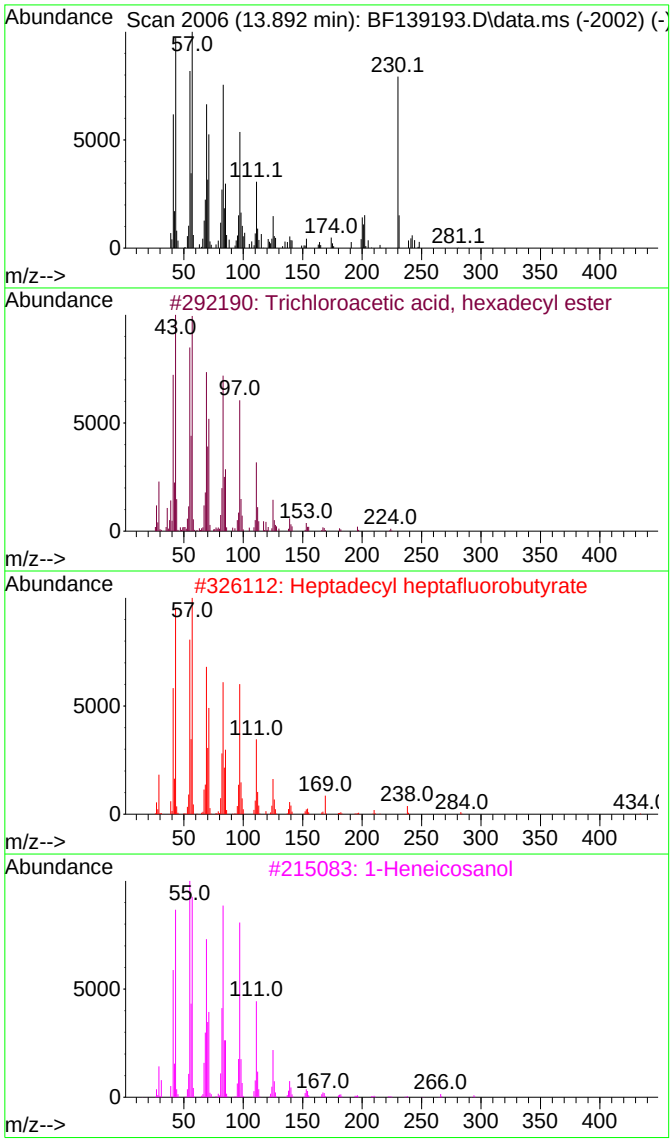
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

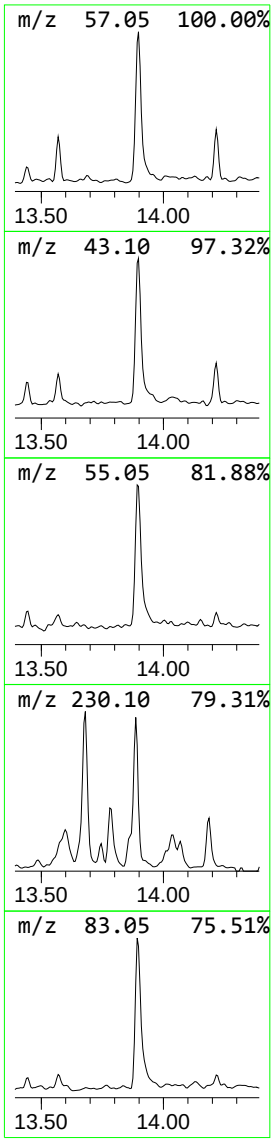
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Trichloroacetic acid, hexad... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	2.35 ng	112833	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
3	1-Heneicosanol	312	C21H44O	015594-90-8	86
4	1-Hexacosene	364	C26H52	018835-33-1	78
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	60





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Data File : BF139193.D
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Operator : RC/JU
Sample : P3739-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.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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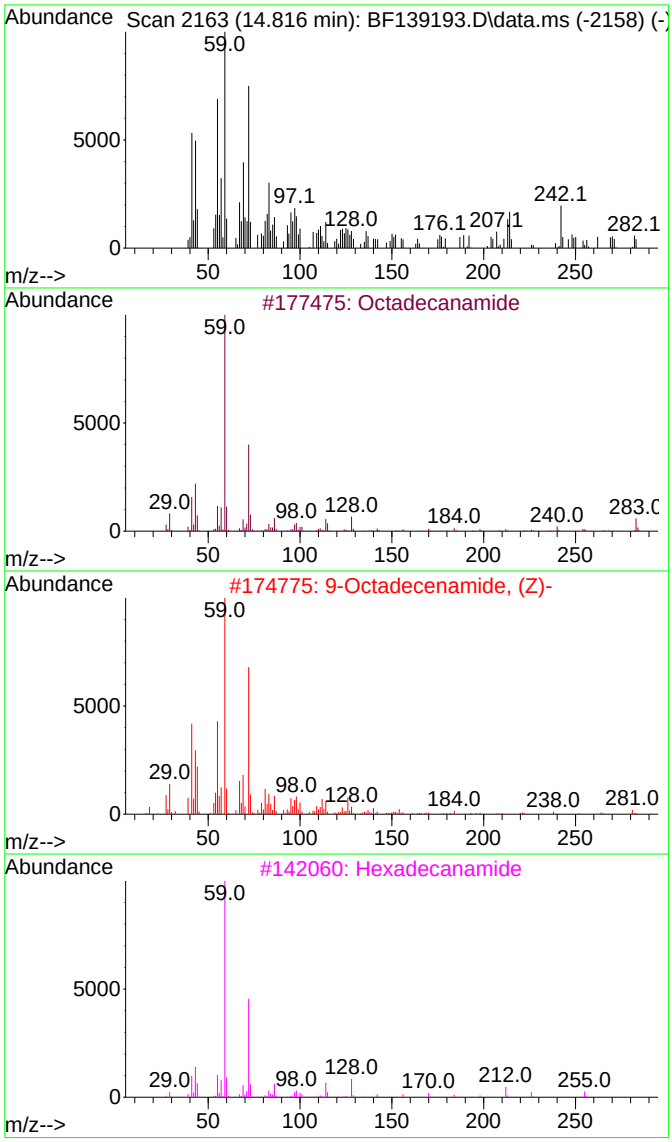
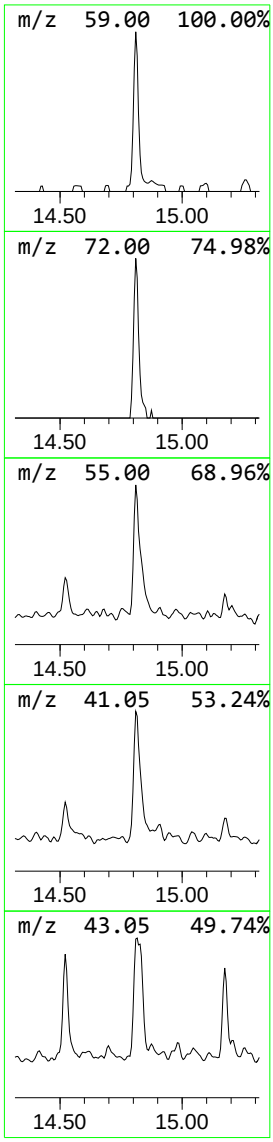
Peak Number 9 Octadecanamide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.816	3.96 ng	95314	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanamide	283	C18H37NO	000124-26-5	62
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	59
3	Hexadecanamide	255	C16H33NO	000629-54-9	53
4	9-Octadecenamide	281	C18H35NO	003322-62-1	46
5	7-Nonenamide	155	C9H17NO	090949-53-4	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139193.D
Acq On : 27 Aug 2024 18:23
Operator : RC/JU
Sample : P3739-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.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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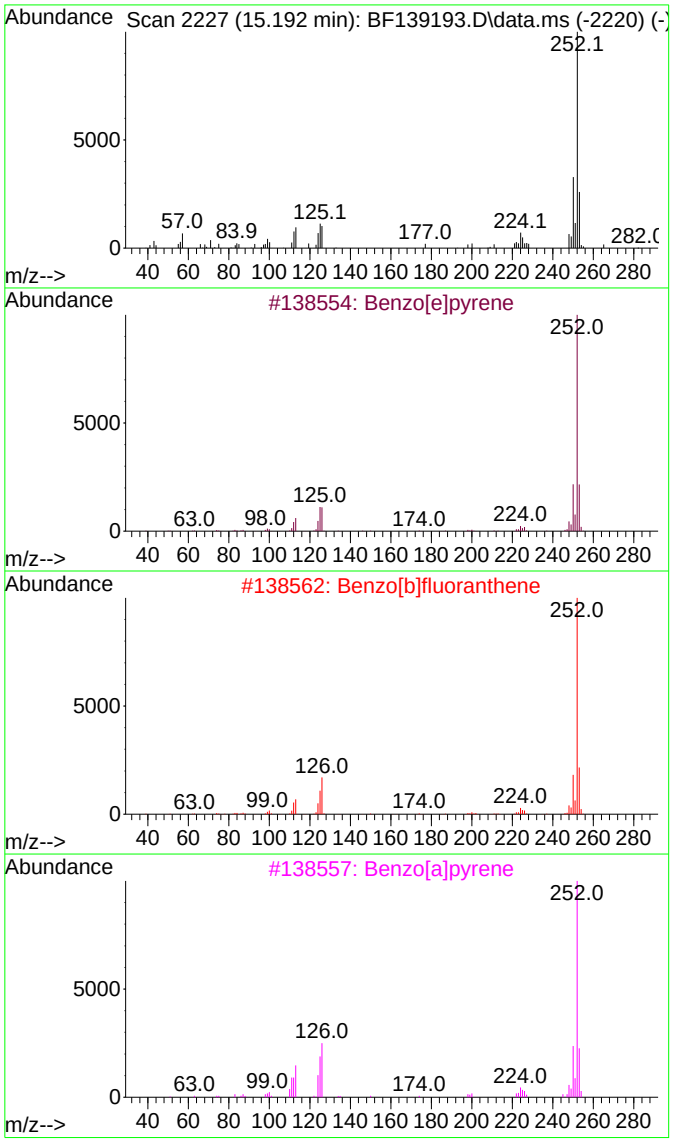
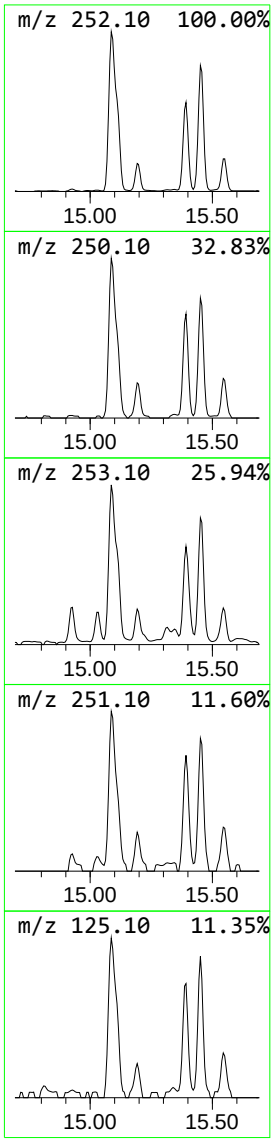
Peak Number 10 Benzo[e]pyrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.192	2.18 ng	52416	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	91
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	90
3	Benzo[a]pyrene	252	C20H12	000050-32-8	81
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	81
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	81





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Data File : BF139193.D
Acq On : 27 Aug 2024 18:23
Operator : RC/JU
Sample : P3739-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.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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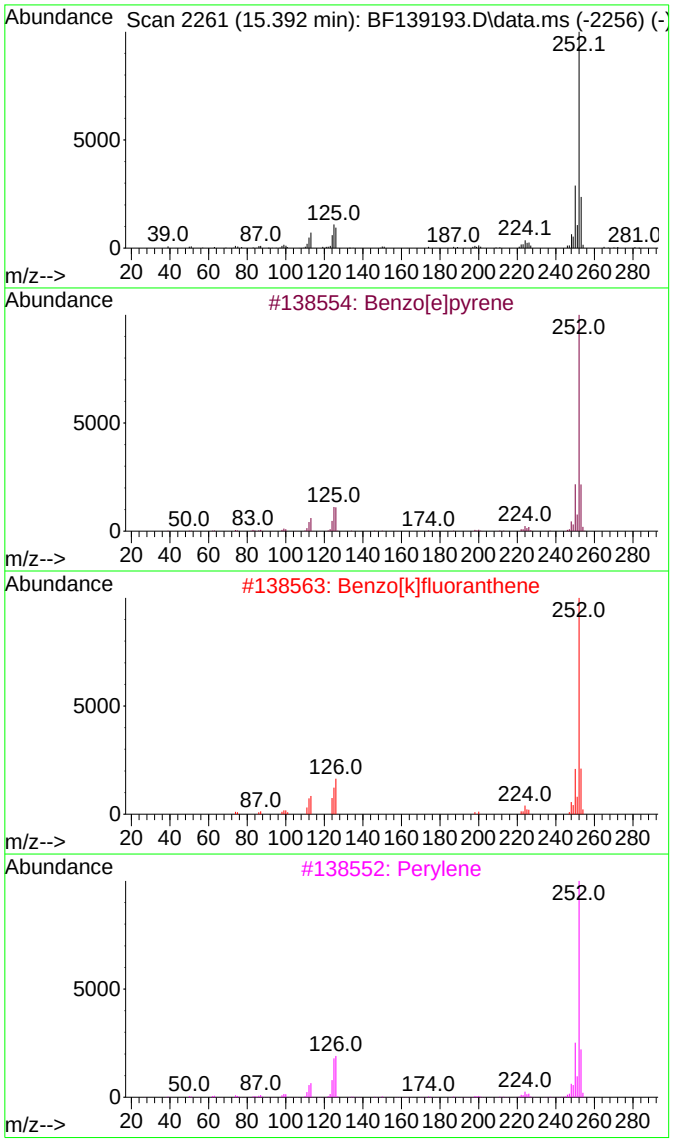
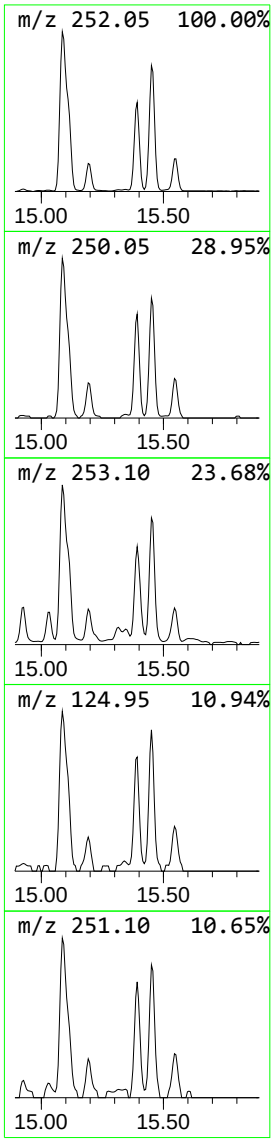
Peak Number 11 Perylene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.392	4.92 ng	118387	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
3	Perylene	252	C20H12	000198-55-0	94
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	94
5	Benzo[a]pyrene	252	C20H12	000050-32-8	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139193.D
Acq On : 27 Aug 2024 18:23
Operator : RC/JU
Sample : P3739-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.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...	2.175	67.7	ng	1714440	1	6.893	506602	20.0
(S)-(+)-1,2-Pro...	3.375	3.8	ng	95261	1	6.893	506602	20.0
2-Pentanone, 4-...	5.099	4.0	ng	102556	1	6.893	506602	20.0
Ethanol, 2-(2-e...	6.710	2.5	ng	64641	1	6.893	506602	20.0
1-Phenoxypropan...	8.481	3.3	ng	106283	2	8.169	647000	20.0
unknown10.022	10.022	58.9	ng	2030170	3	9.922	689878	20.0
Anthracene, 2-m...	11.933	3.4	ng	139807	4	11.410	818812	20.0
Trichloroacetic...	13.892	2.4	ng	112833	5	14.045	962228	20.0
Octadecanamide	14.816	4.0	ng	95314	6	15.515	481177	20.0
Benzo[e]pyrene	15.192	2.2	ng	52416	6	15.515	481177	20.0
Perylene	15.392	4.9	ng	118387	6	15.515	481177	20.0