LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072524\
Data File : BF138659.D
Acq On : 25 Jul 2024 18:21
Operator : RC/JU
Sample : P3357-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-857-J-SO-1.5-2-072024

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-BF070924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138659.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	3	8	21	rVB	994912	1525798	79.23%	9.906%
2	3.369	210	217	234	rBV	48022	115157	5.98%	0.748%
3	5.075	502	507	520	rVB	90325	134389	6.98%	0.872%
4	5.481	570	576	591	rBV	1393556	1820180	94.51%	11.817%
5	6.487	741	747	773	rVB	1413276	1923764	99.89%	12.489%
6	6.681	775	780	792	rVB	56014	76790	3.99%	0.499%
7	6.851	804	809	814	rBV	359685	431681	22.41%	2.803%
8	7.416	898	905	910	rBV	920765	1222794	63.49%	7.939%
9	7.669	943	948	958	rVB	21550	28512	1.48%	0.185%
10	8.134	1021	1027	1032	rBV	473498	587979	30.53%	3.817%
11	8.445	1075	1080	1098	rBV	126794	183638	9.54%	1.192%
12	9.204	1203	1209	1220	rBV	1472363	1925884	100.00%	12.503%
13	9.886	1319	1325	1335	rVB	519963	661250	34.33%	4.293%
14	9.975	1335	1340	1349	rBV	134436	208149	10.81%	1.351%
15	10.675	1453	1459	1474	rBV	893944	1189367	61.76%	7.721%
16	11.369	1572	1577	1586	rBV2	466608	691913	35.93%	4.492%
17	11.757	1638	1643	1649	rVB	17816	21195	1.10%	0.138%
18	11.898	1659	1667	1678	rBV3	34807	75242	3.91%	0.488%
19	11.980	1678	1681	1690	rVB	11365	19737	1.02%	0.128%
20	12.463	1759	1763	1768	rVB3	14180	21842	1.13%	0.142%
21	12.580	1779	1783	1788	rBB	80145	94808	4.92%	0.616%
22	12.810	1813	1822	1826	rBV	62501	92083	4.78%	0.598%
23	12.951	1841	1846	1851	rBV	957618	1202439	62.44%	7.806%
24	13.851	1994	1999	2015	rVB	61588	133797	6.95%	0.869%
25	14.004	2019	2025	2036	rVB	273557	409033	21.24%	2.655%
26	14.468	2099	2104	2106	rBV	17459	26701	1.39%	0.173%
27	14.680	2136	2140	2145	rBV4	13974	21119	1.10%	0.137%
28	15.045	2198	2202	2209	rVV2	21746	44286	2.30%	0.288%
29	15.104	2209	2212	2217	rVB	19407	26338	1.37%	0.171%
30	15.351	2248	2254	2259	rBV2	18440	39199	2.04%	0.254%
31	15.404	2259	2263	2268	rVB	19746	30541	1.59%	0.198%
32	15.468	2268	2274	2287	rBV	233787	371997	19.32%	2.415%
33	15.915	2346	2350	2358	rVB3	15572	26340	1.37%	0.171%
34	15.998	2358	2364	2366	rBV7	9363	19384	1.01%	0.126%

Sum of corrected areas: 15403326

Instrument :
BNA_F
ClientSampleId :
S-857-J-SO-1.5-2-072024

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072524\
Data File : BF138659.D
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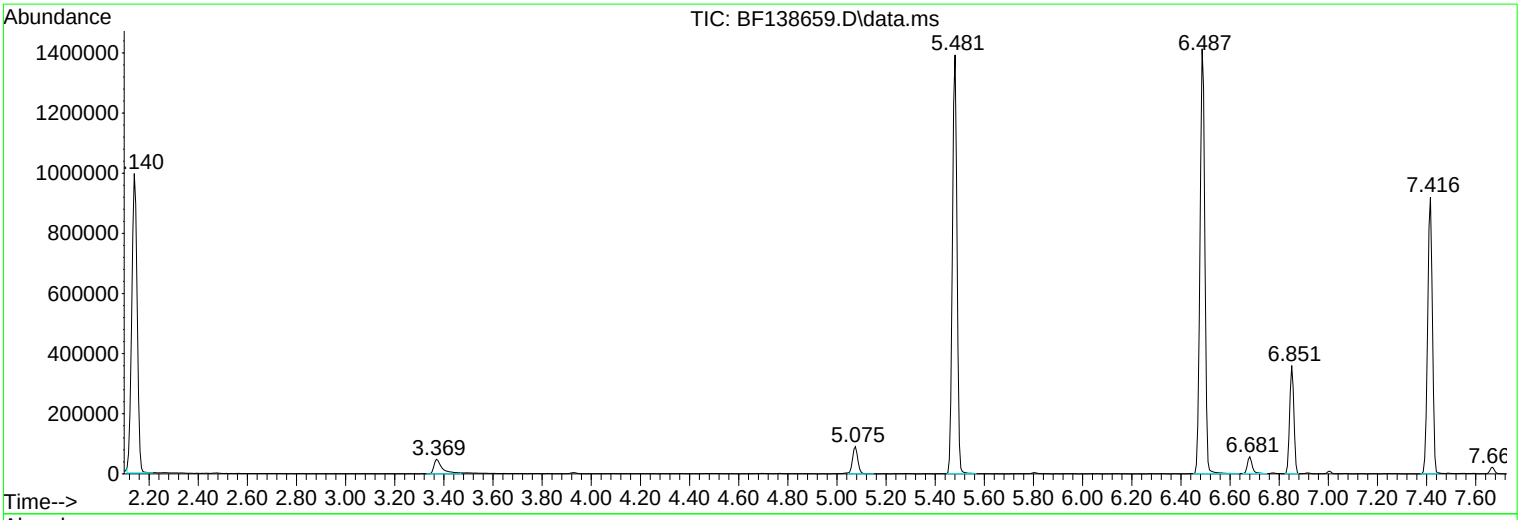
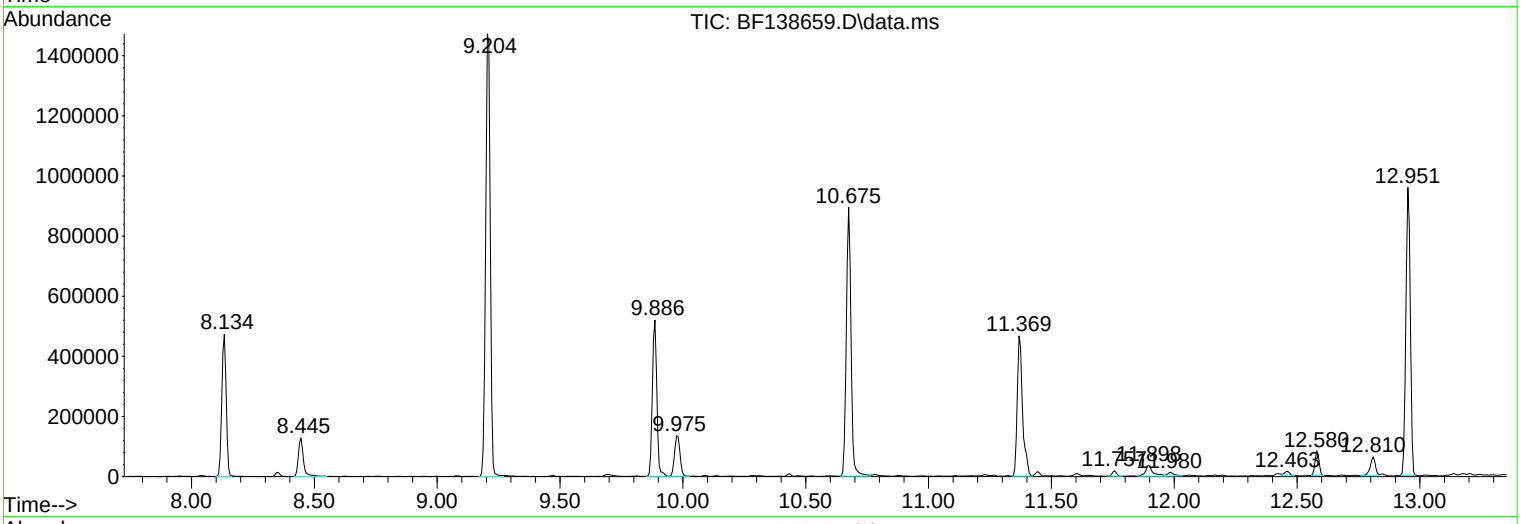
Misc :
ALS Vial : 13 Sample Multiplier: 1

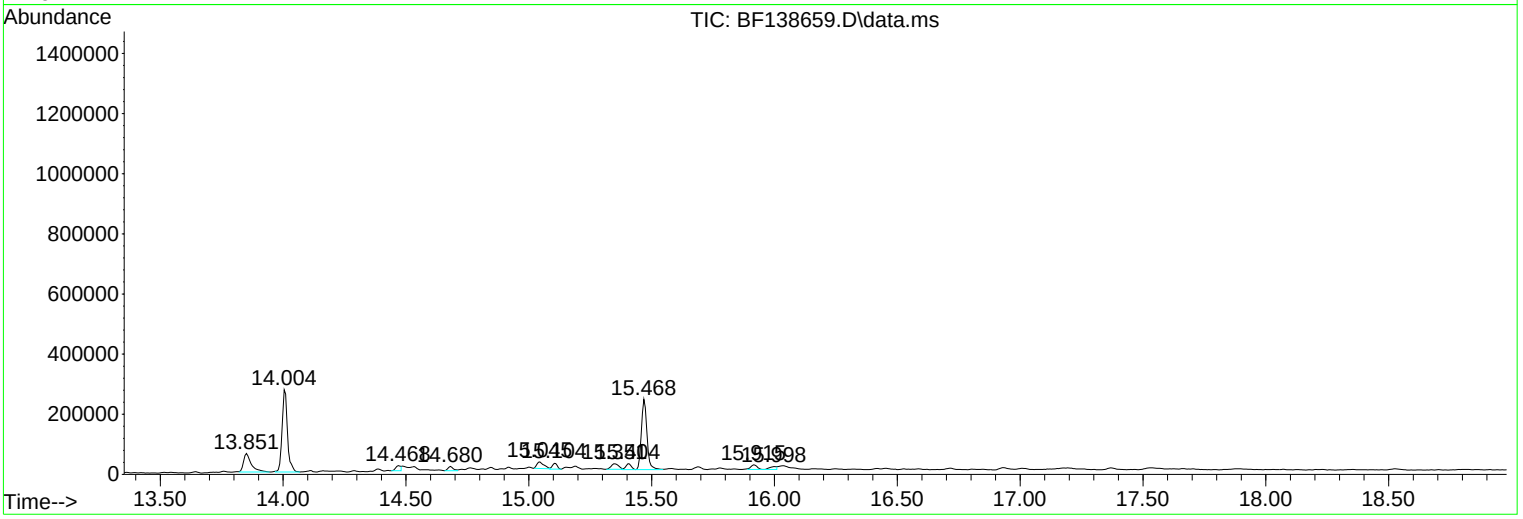
Instrument :
BNA_F
ClientSampleId :
S-857-J-SO-1.5-2-072024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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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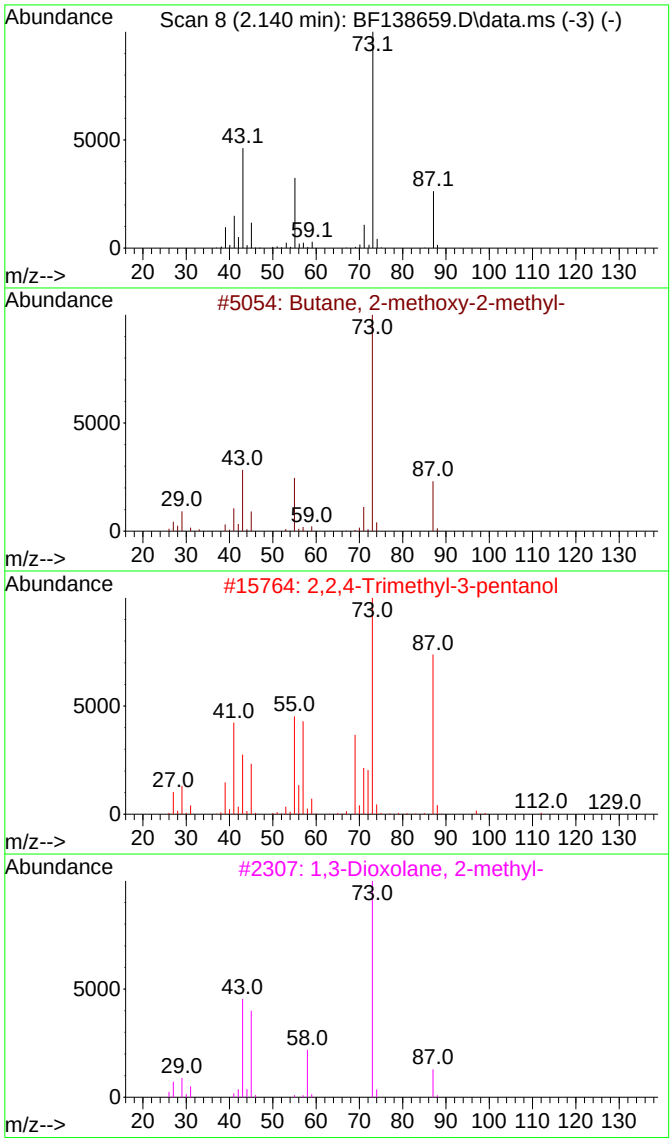
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

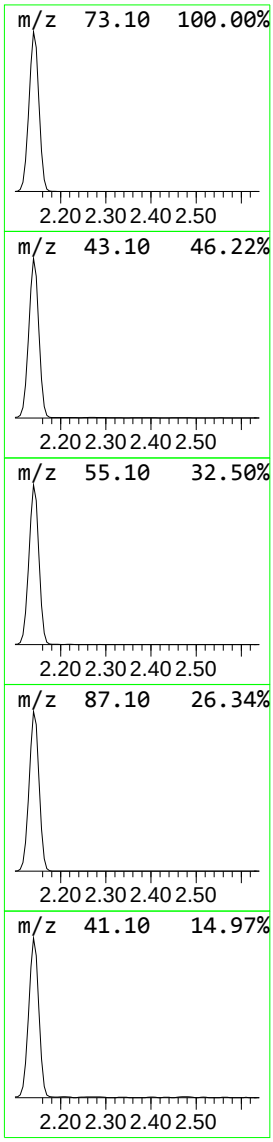
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	70.69 ng	1525800	1,4-Dichlorobenzene-d4	6.851

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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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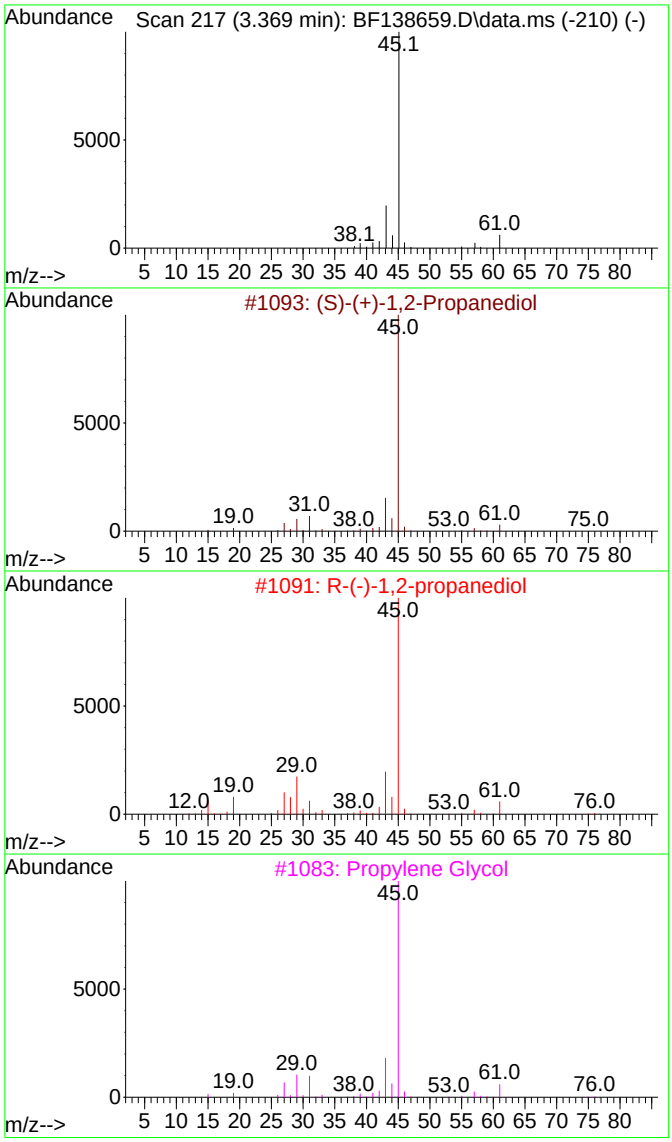
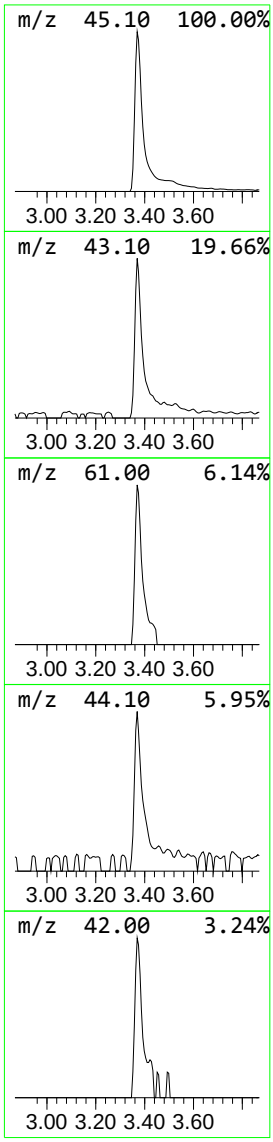
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.369	5.34 ng	115157	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	74
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
3	Propylene Glycol	76	C3H8O2	000057-55-6	43
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9





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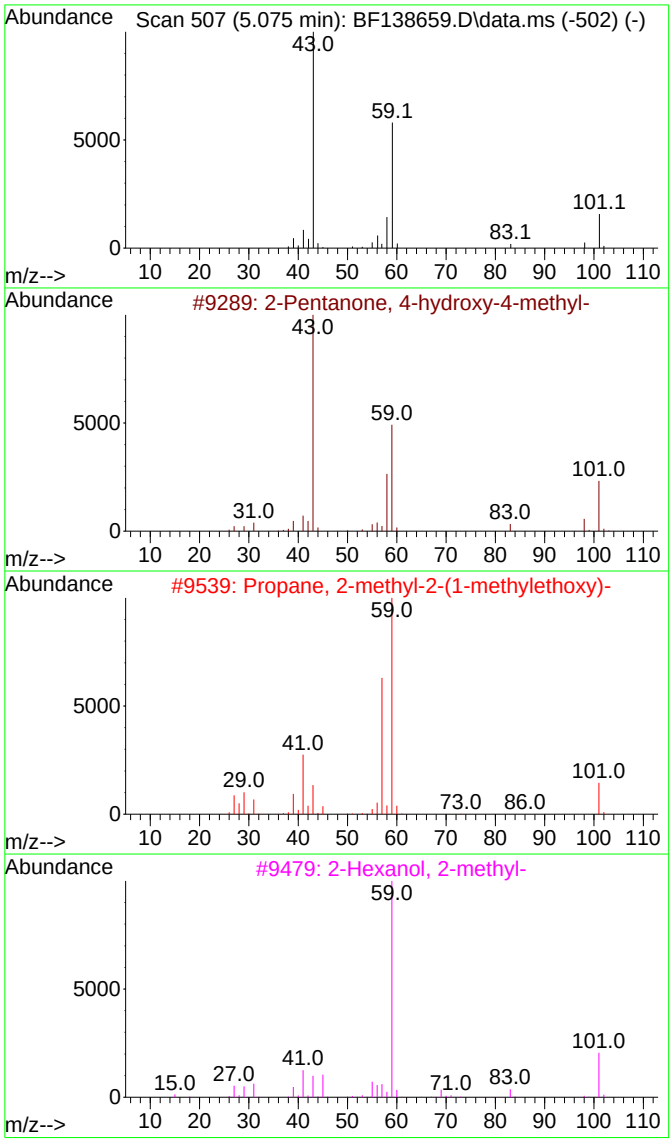
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

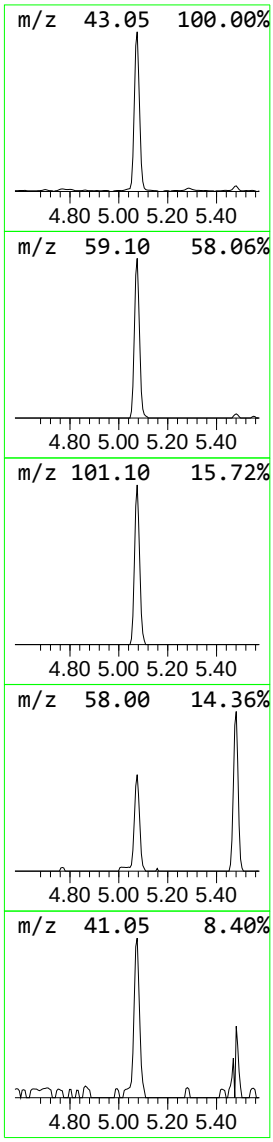
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	6.23 ng	134389	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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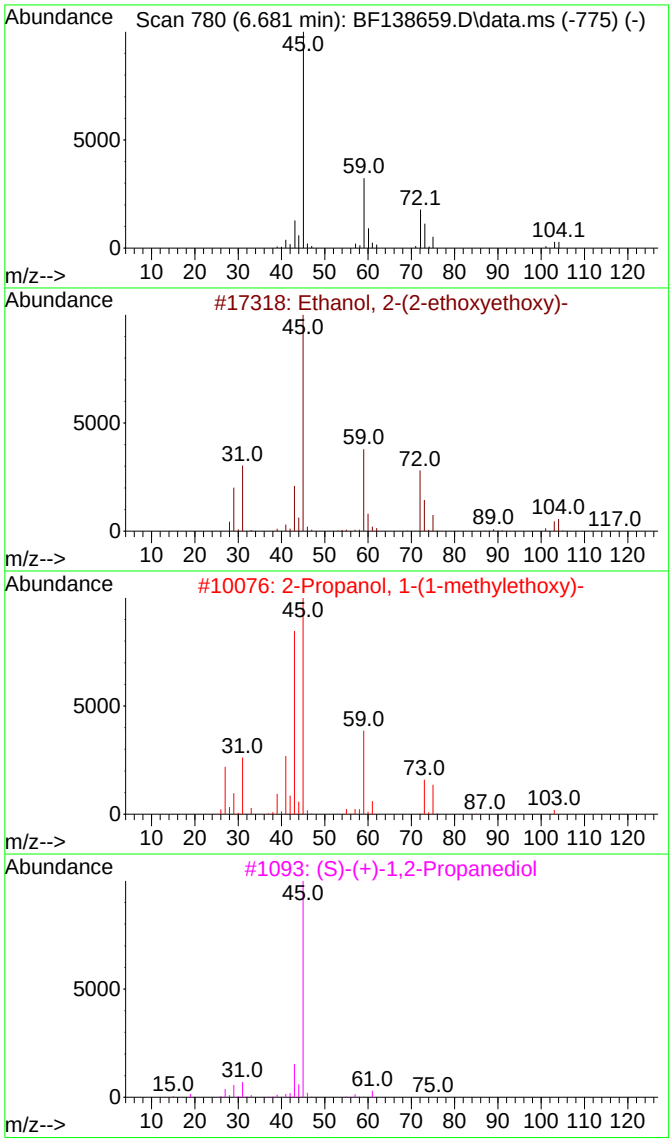
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

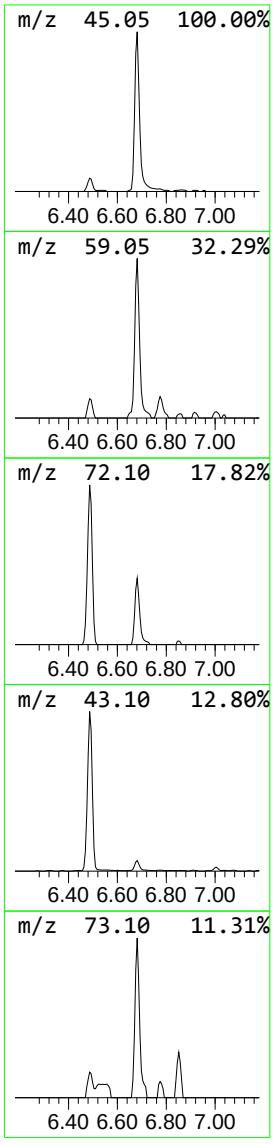
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.681	3.56 ng	76790	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	39
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	37
4	Methoxyacetic acid, butyl ester	146	C7H14O3	017640-22-1	33
5	Ethyl ether	74	C4H10O	000060-29-7	33





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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

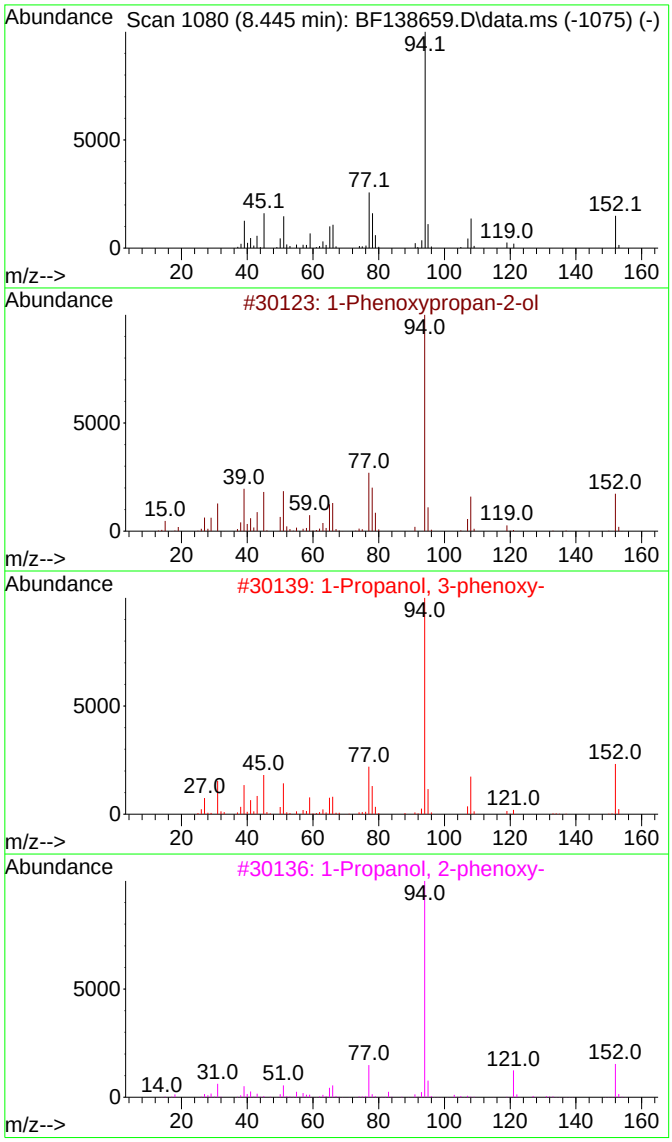
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

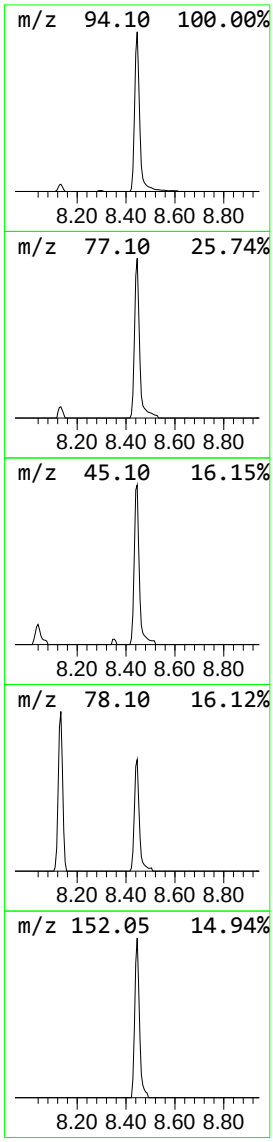
****

Peak Number 5 1-Phenoxypropan-2-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.445	6.25 ng	183638	Naphthalene-d8	8.134

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	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
4	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
5	Benzene, (1,1-dimethylethoxy)-	150	C10H14O	006669-13-2	53





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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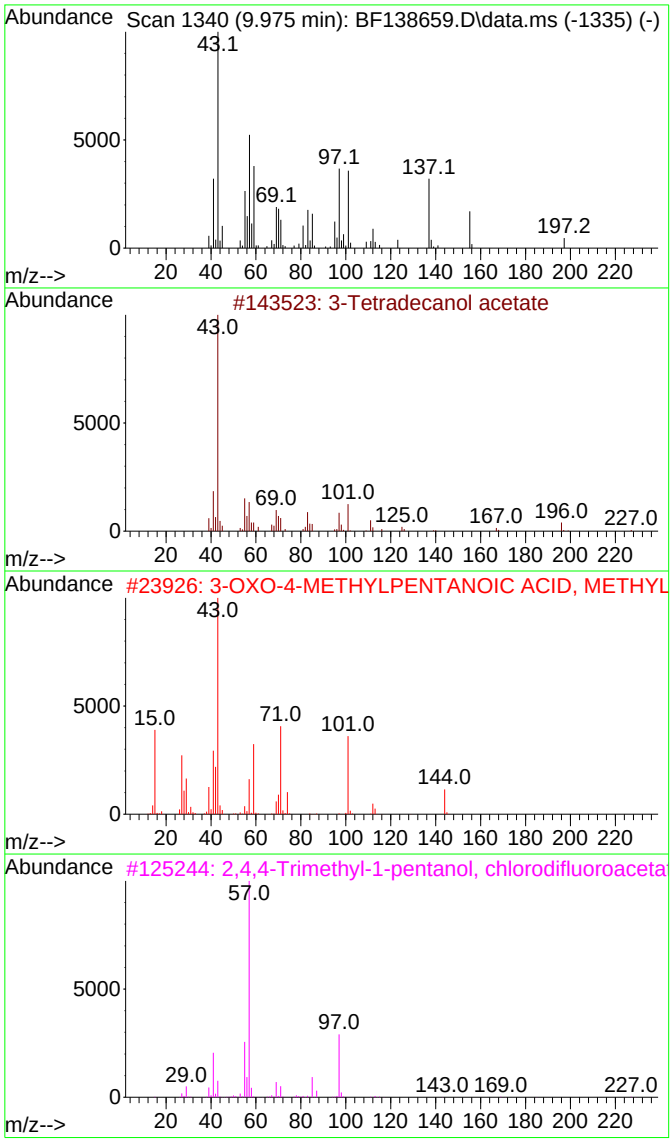
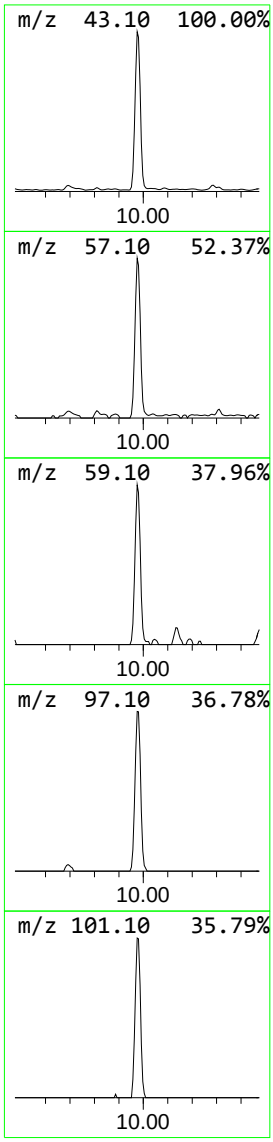
****

Peak Number 6 unknown9.975 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.975	6.30 ng	208149	Acenaphthene-d10	9.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Tetradecanol acetate	256	C16H32O2	051354-23-5	25
2	3-OXO-4-METHYLPENTANOIC ACID, ME...	144	C7H12O3	042558-54-3	10
3	2,4,4-Trimethyl-1-pentanol, chlo...	242	C10H17ClF2O2	1000447-27-2	10
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	10
5	2-Piperidinone, N-[4-bromo-n-but...	233	C9H16BrNO	195194-80-0	10





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TIC Library : C:\Database\NIST20.L
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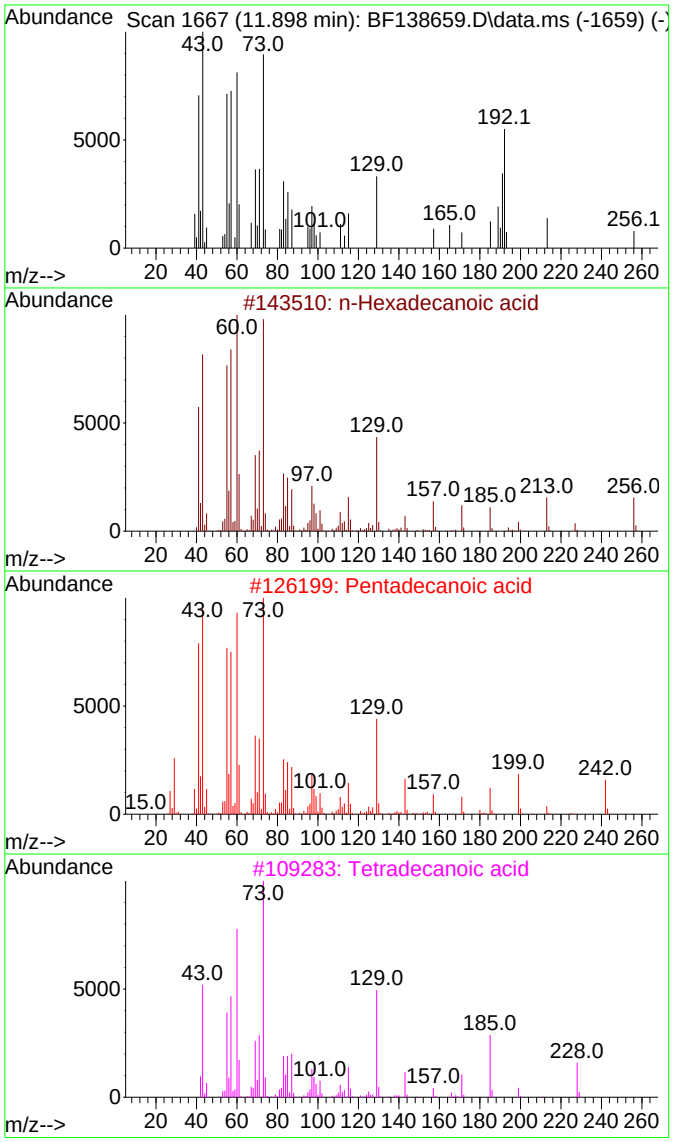
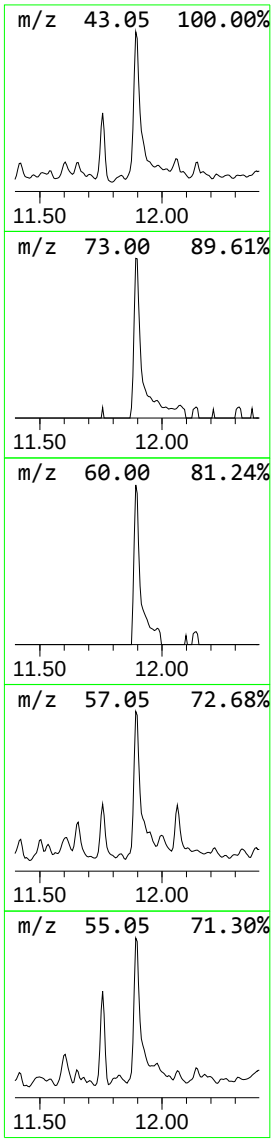
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	2.17 ng	75242	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	47
4	n-Decanoic acid	172	C10H20O2	000334-48-5	38
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	22





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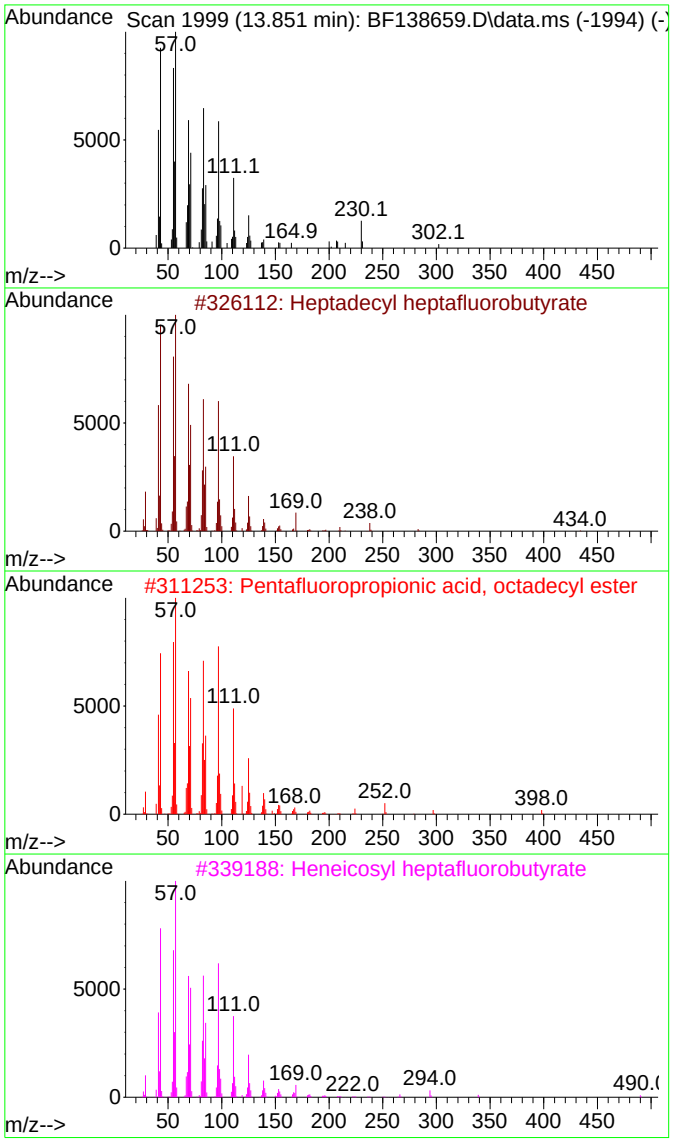
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

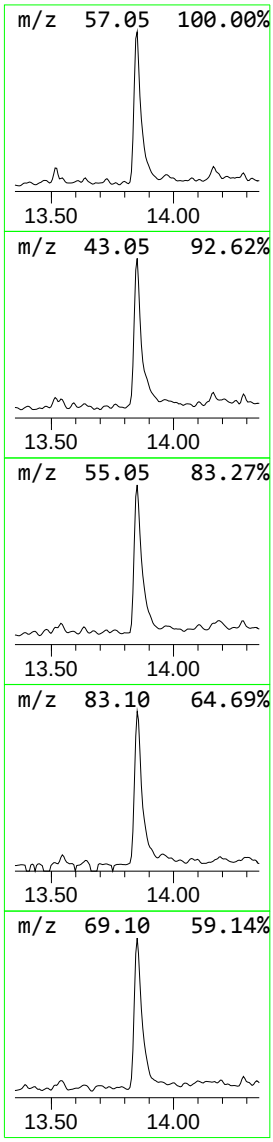
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Heptadecyl heptafluorobutyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.851	6.54 ng	133797	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
2	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
3	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	90
4	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	90
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90





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Sample : P3357-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

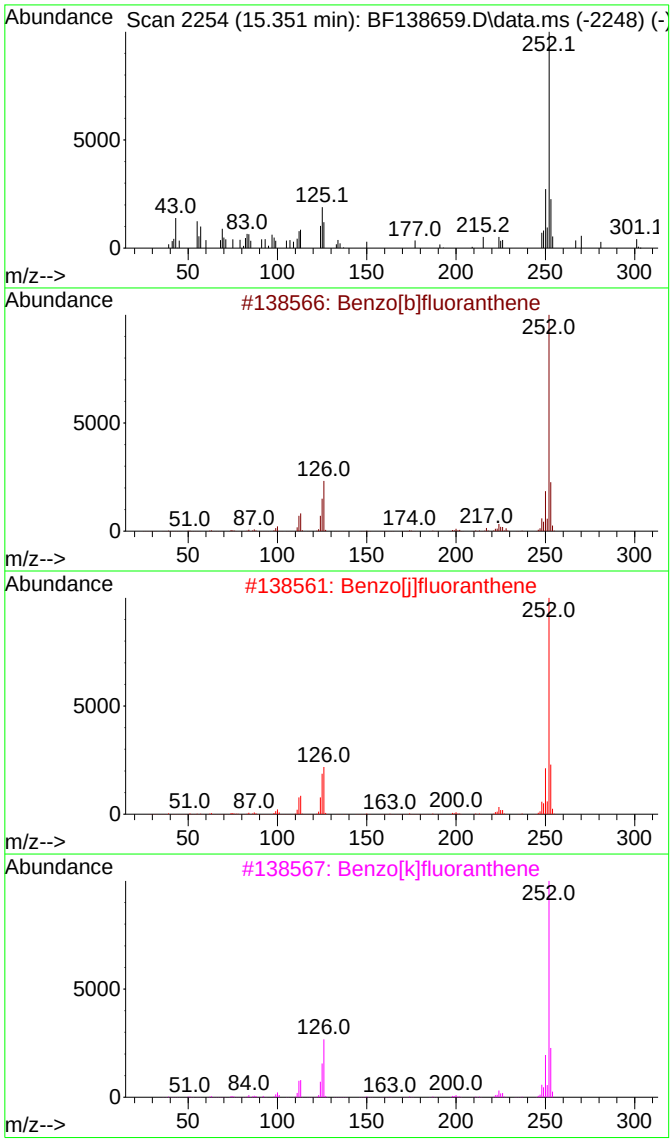
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

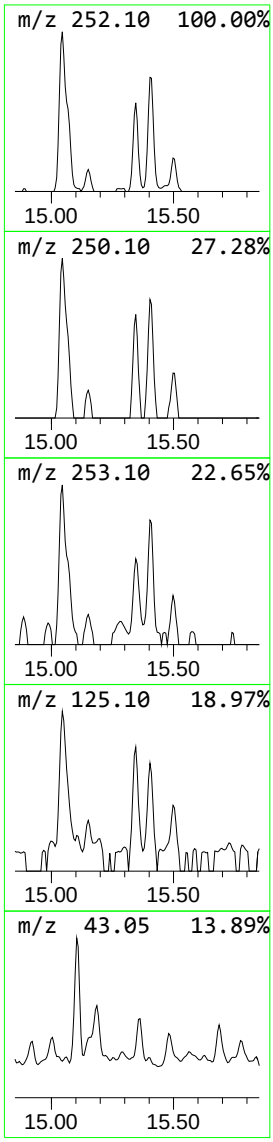
****

Peak Number 9 Benzo[j]fluoranthene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.351	2.11 ng	39199	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]fluoranthene	252	C20H12	000205-99-2	89
2	Benzo[j]fluoranthene	252	C20H12	000205-82-3	89
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	89
4	Benzo[a]pyrene	252	C20H12	000050-32-8	81
5	Benzo[e]pyrene	252	C20H12	000192-97-2	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072524\
Data File : BF138659.D
Acq On : 25 Jul 2024 18:21
Operator : RC/JU
Sample : P3357-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-857-J-SO-1.5-2-072024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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...	2.140	70.7	ng	1525800	1	6.851	431681	20.0
(S)-(+)-1,2-Pro...	3.369	5.3	ng	115157	1	6.851	431681	20.0
2-Pentanone, 4-...	5.075	6.2	ng	134389	1	6.851	431681	20.0
Ethanol, 2-(2-e...	6.681	3.6	ng	76790	1	6.851	431681	20.0
1-Phenoxypropan...	8.445	6.3	ng	183638	2	8.134	587979	20.0
unknown9.975	9.975	6.3	ng	208149	3	9.886	661250	20.0
n-Hexadecanoic ...	11.898	2.2	ng	75242	4	11.369	691913	20.0
Heptadecyl hept...	13.851	6.5	ng	133797	5	14.004	409033	20.0
Benzo[j]fluoran...	15.351	2.1	ng	39199	6	15.468	371997	20.0