LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052824\
Data File : BF138049.D
Acq On : 28 May 2024 16:07
Operator : CG\JU
Sample : P2616-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-206

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-BF051424.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138049.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	12	16	23	rVB2	36619	67835	2.53%	0.290%
2	2.404	46	54	59	rBV	1211259	1644896	61.32%	7.031%
3	3.693	271	273	285	rBV5	15462	34327	1.28%	0.147%
4	5.281	539	543	549	rVB	54526	67175	2.50%	0.287%
5	5.663	604	608	611	rBV	2446615	2292670	85.46%	9.800%
6	6.651	771	776	779	rBV	2280720	2242703	83.60%	9.587%
7	6.739	788	791	794	rVB	41710	31782	1.18%	0.136%
8	7.033	838	841	845	rBV	1076145	829022	30.90%	3.544%
9	7.598	932	937	940	rBV	1624198	1465467	54.63%	6.264%
10	7.833	973	977	982	rBV	82155	68497	2.55%	0.293%
11	8.204	1037	1040	1051	rBV	109199	138123	5.15%	0.590%
12	8.316	1056	1059	1063	rBV	1209706	1050489	39.16%	4.490%
13	8.622	1108	1111	1125	rBV	56405	81060	3.02%	0.346%
14	9.392	1238	1242	1245	rBV	3325949	2682673	100.00%	11.467%
15	10.080	1356	1359	1363	rBV	1256805	1006545	37.52%	4.303%
16	10.116	1363	1365	1368	rVV	74270	59551	2.22%	0.255%
17	10.163	1368	1373	1381	rVB2	59093	83881	3.13%	0.359%
18	10.633	1449	1453	1456	rBV	47308	44353	1.65%	0.190%
19	10.874	1490	1494	1507	rBV	1326119	1232531	45.94%	5.269%
20	11.574	1610	1613	1616	rBV	873244	837715	31.23%	3.581%
21	11.598	1616	1617	1621	rVV	409954	313065	11.67%	1.338%
22	11.651	1621	1626	1630	rVV	57254	53220	1.98%	0.227%
23	11.810	1647	1653	1657	rBV2	33371	47952	1.79%	0.205%
24	12.086	1695	1700	1702	rBV	390340	399531	14.89%	1.708%
25	12.110	1702	1704	1709	rVB	92180	89524	3.34%	0.383%
26	12.192	1715	1718	1721	rBV2	72686	87573	3.26%	0.374%
27	12.398	1751	1753	1758	rVB	50674	52838	1.97%	0.226%
28	12.627	1789	1792	1795	rBV	26863	32278	1.20%	0.138%
29	12.798	1815	1821	1825	rBV	633011	576089	21.47%	2.463%
30	12.868	1829	1833	1839	rBV3	190879	233251	8.69%	0.997%
31	13.010	1854	1857	1858	rBV2	94249	93361	3.48%	0.399%
32	13.027	1858	1860	1865	rVB	502083	430445	16.05%	1.840%
33	13.074	1865	1868	1872	rVB2	33792	33867	1.26%	0.145%
34	13.162	1879	1883	1886	rBV	2426652	2030635	75.69%	8.680%
35	13.245	1893	1897	1900	rBV2	25776	37998	1.42%	0.162%
36	13.357	1913	1916	1918	rVB2	62935	53969	2.01%	0.231%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052824\
Data File : BF138049.D
Acq On : 28 May 2024 16:07
Operator : CG\JU
Sample : P2616-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-206

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-BF051424.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.421	1924	1927	1930	rVB2	46624	36742	1.37%	0.157%
38	13.462	1930	1934	1936	rBV2	51801	61015	2.27%	0.261%
39	13.662	1966	1968	1971	rBV	41207	39014	1.45%	0.167%
40	13.862	2000	2002	2005	rVB	52242	45246	1.69%	0.193%
41	14.057	2032	2035	2043	rVB4	137468	276192	10.30%	1.181%
42	14.227	2059	2064	2067	rBV2	930175	1068554	39.83%	4.568%
43	14.257	2067	2069	2076	rVB	252842	228134	8.50%	0.975%
44	15.321	2247	2250	2254	rBV	174250	262909	9.80%	1.124%
45	15.656	2304	2307	2313	rVB	99142	123589	4.61%	0.528%
46	15.727	2315	2319	2325	rBV	130623	179790	6.70%	0.769%
47	15.798	2327	2331	2335	rVV	455578	546159	20.36%	2.335%

Sum of corrected areas: 23394235

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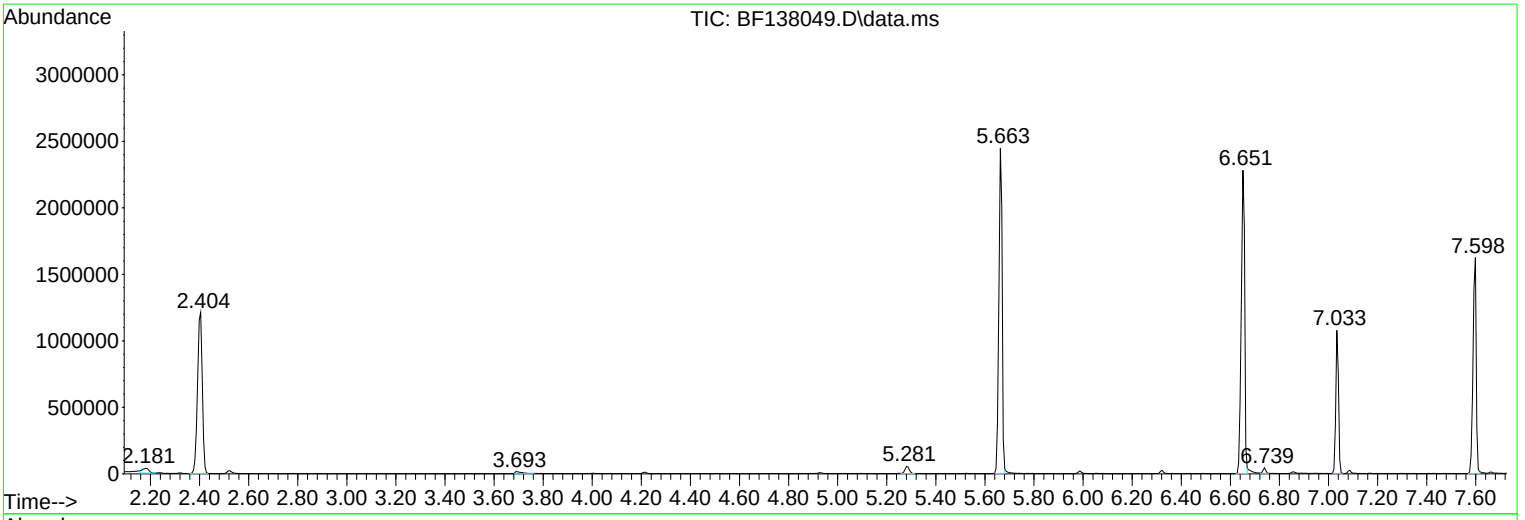
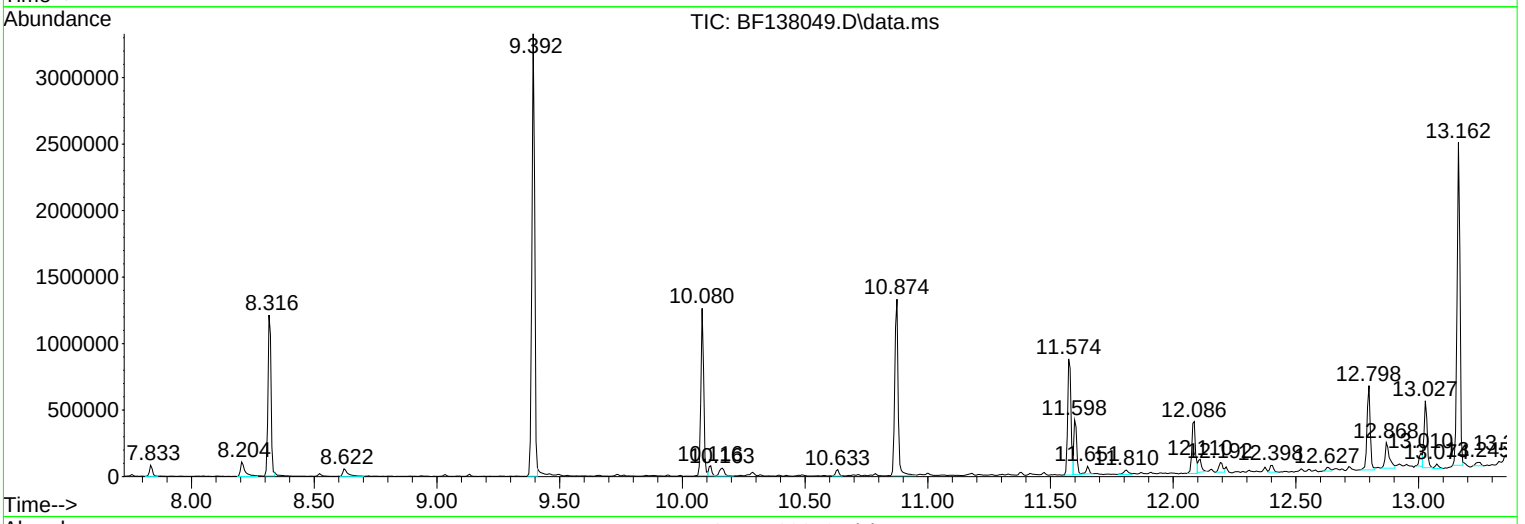
Misc :
ALS Vial : 13 Sample Multiplier: 1

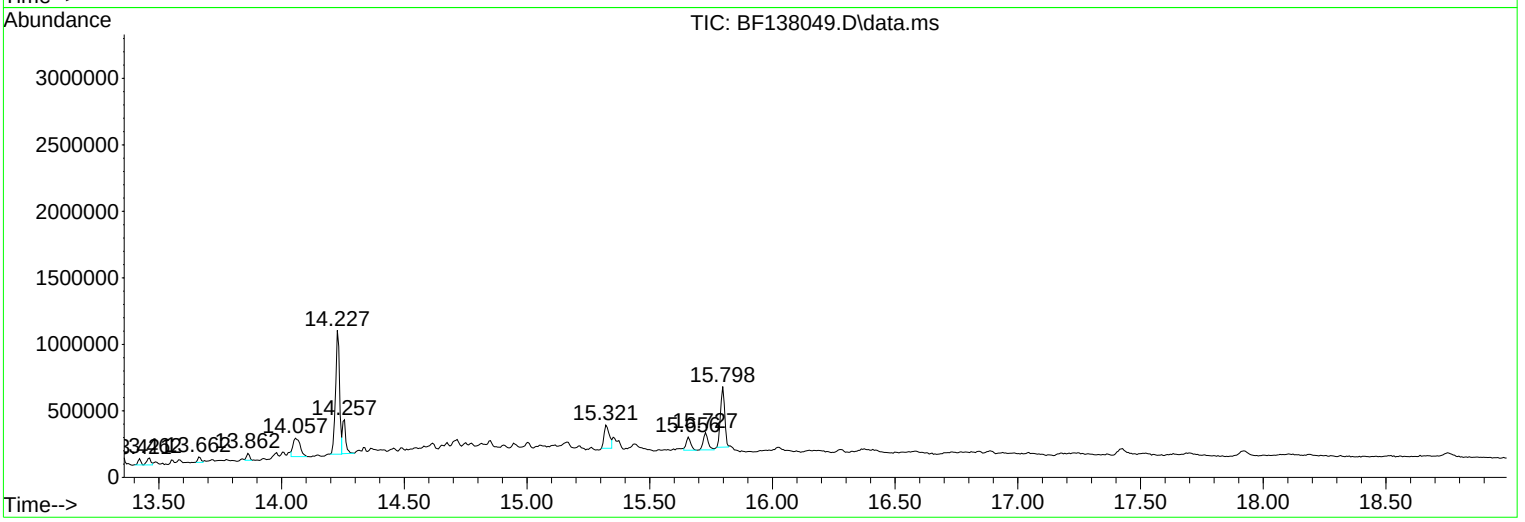
Instrument :
BNA_F
ClientSampleId :
VNJ-206

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF051424.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\BF052824\
Data File : BF138049.D
Acq On : 28 May 2024 16:07
Operator : CG\JU
Sample : P2616-01
Misc :
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Instrument :
BNA_F
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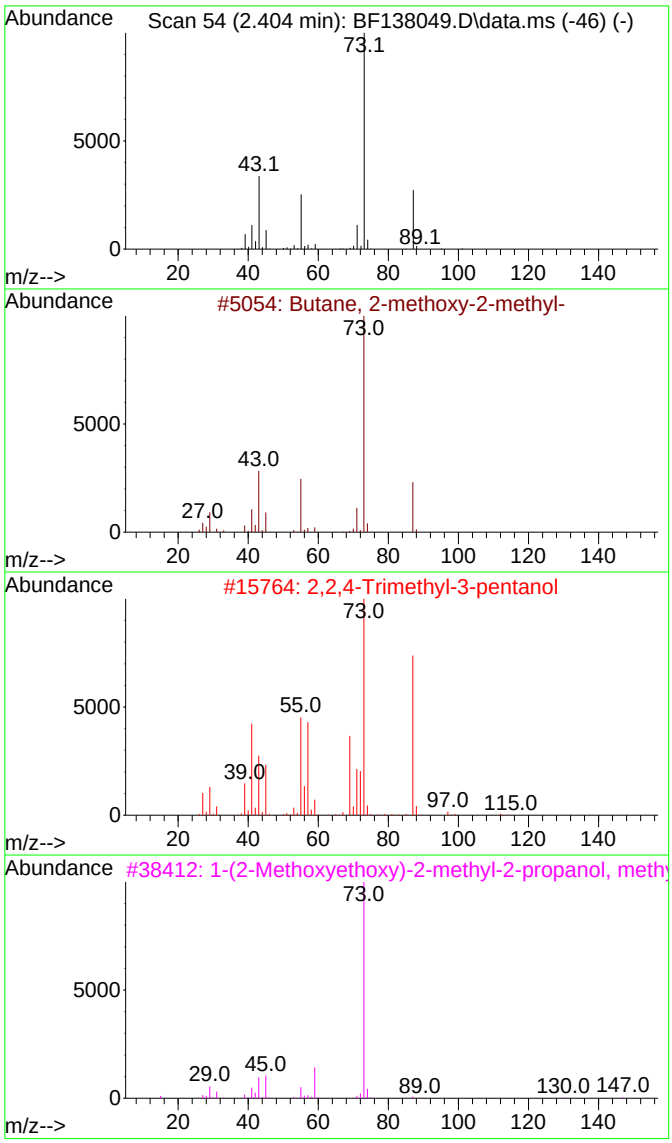
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF051424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

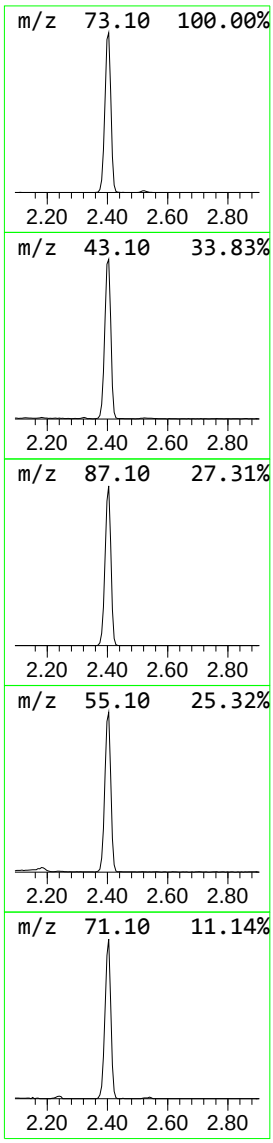
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.404	39.68 ng	1644900	1,4-Dichlorobenzene-d4	7.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





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Data File : BF138049.D
Acq On : 28 May 2024 16:07
Operator : CG\JU
Sample : P2616-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-206

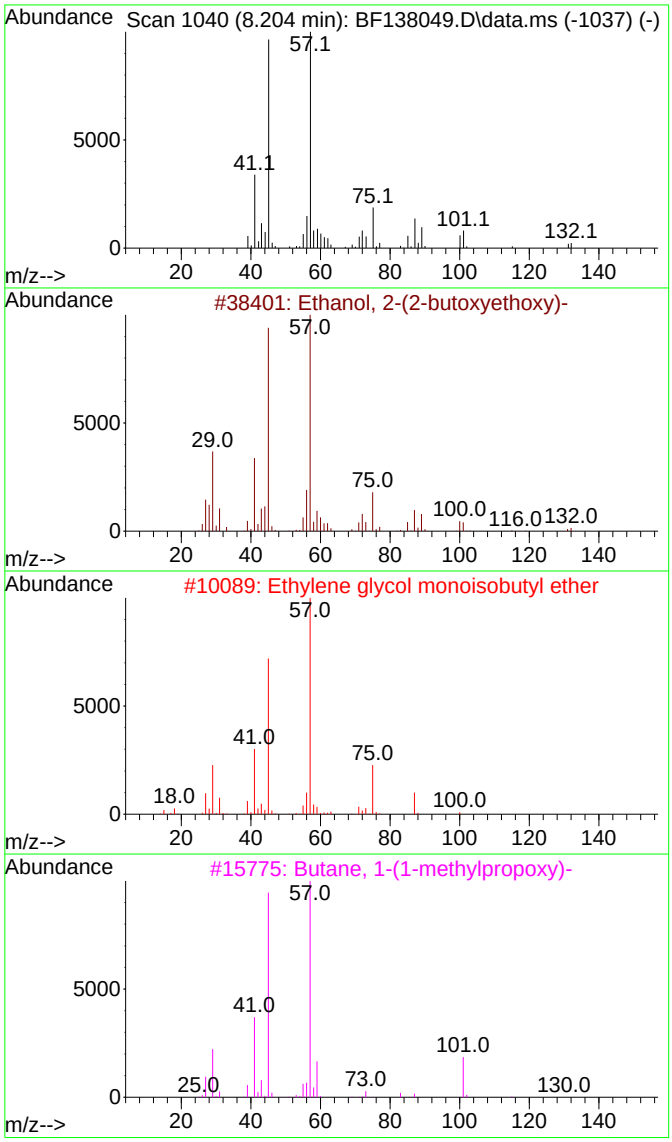
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF051424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

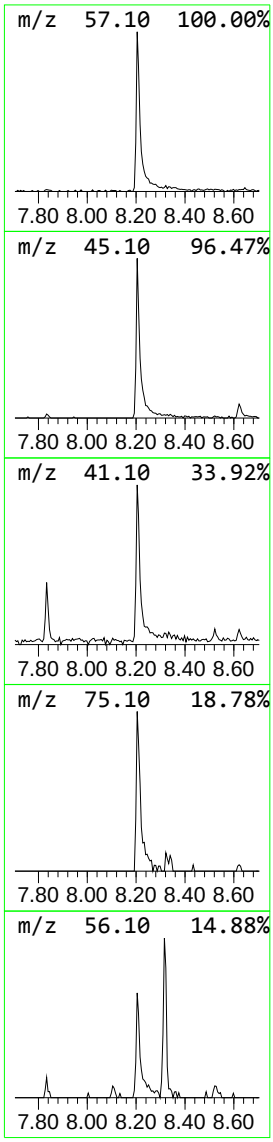
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.204	2.63 ng	138123	Naphthalene-d8	8.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
3	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
4	Methoxyacetic acid, butyl ester	146	C7H14O3	017640-22-1	53
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53





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Data File : BF138049.D
Acq On : 28 May 2024 16:07
Operator : CG\JU
Sample : P2616-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-206

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF051424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

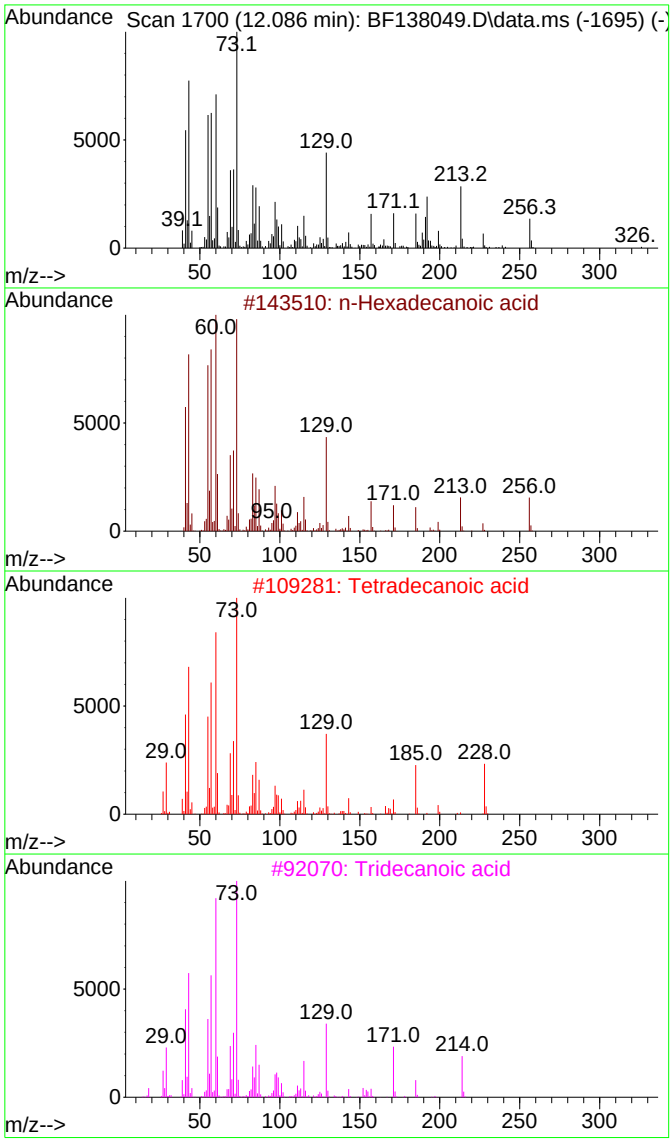
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

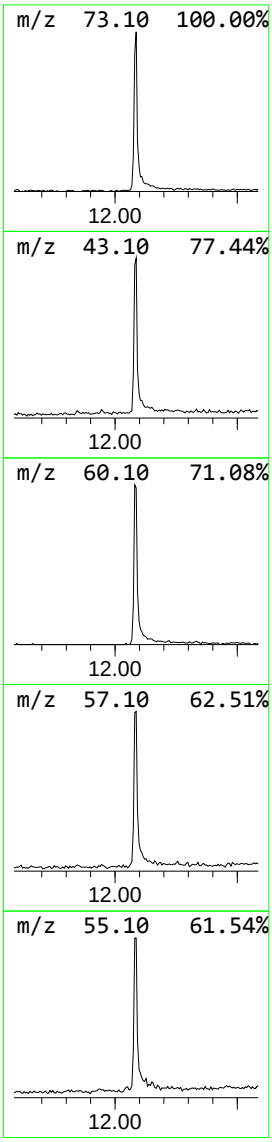
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.086	9.54 ng	399531	Phenanthrene-d10	11.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3	Tridecanoic acid	214	C13H26O2	000638-53-9	86
4	Dodecanoic acid	200	C12H24O2	000143-07-7	64
5	Octadecanoic acid	284	C18H36O2	000057-11-4	64





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Data File : BF138049.D
Acq On : 28 May 2024 16:07
Operator : CG\JU
Sample : P2616-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-206

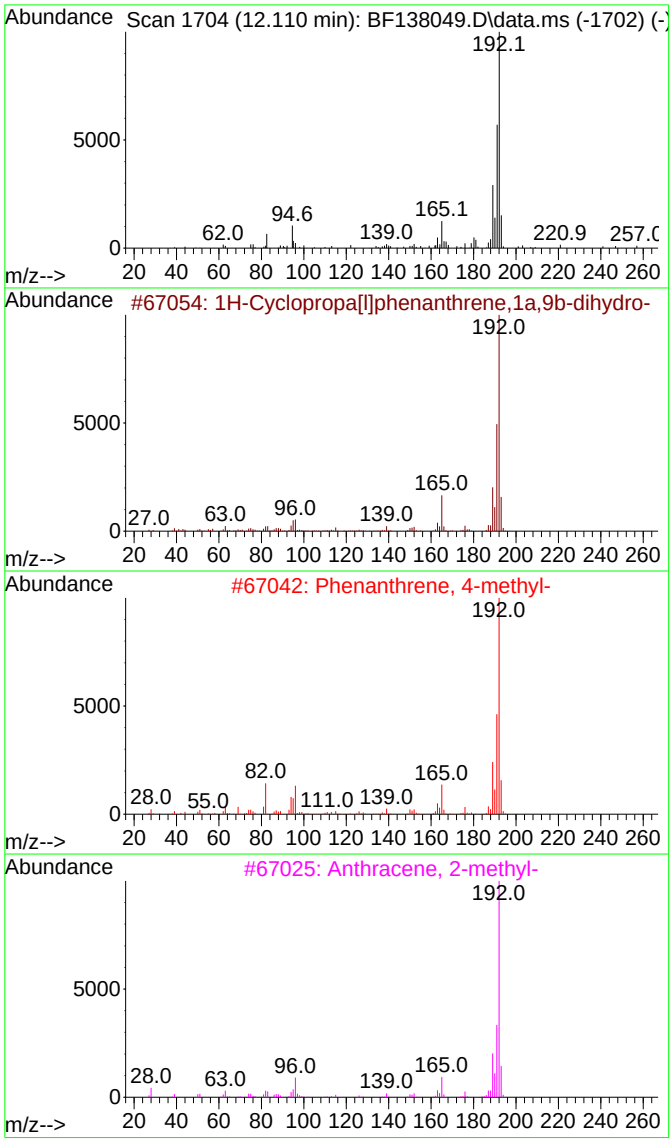
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF051424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

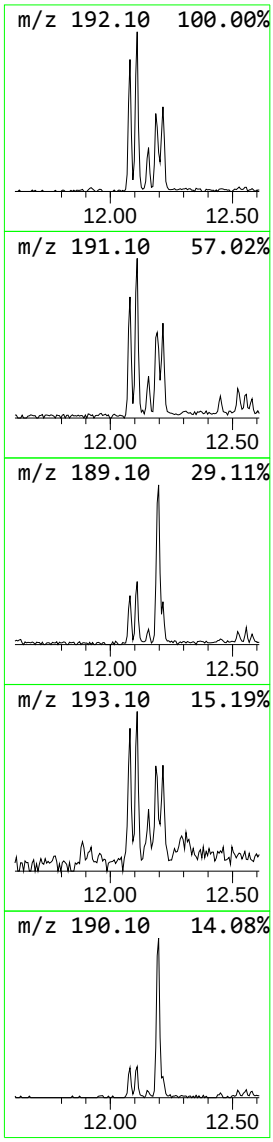
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1H-Cyclopropa[l]phenanthren... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.110	2.14 ng	89524	Phenanthrene-d10	11.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	90
2	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	87
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	86
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	81
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	81





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Data File : BF138049.D
Acq On : 28 May 2024 16:07
Operator : CG\JU
Sample : P2616-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-206

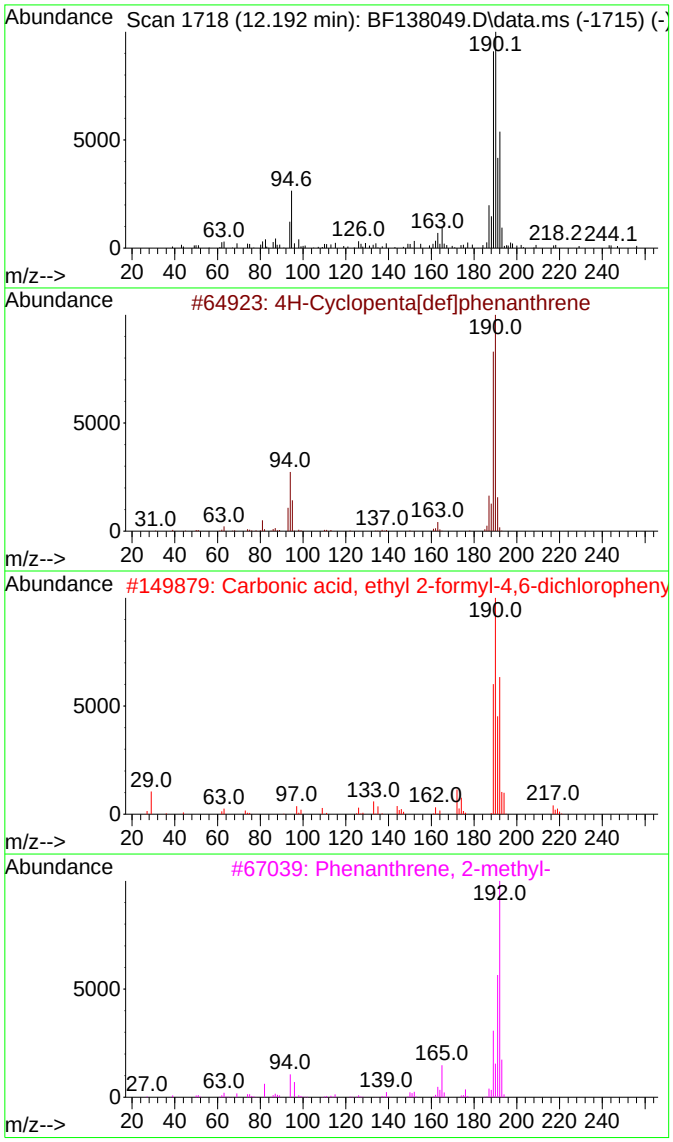
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF051424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

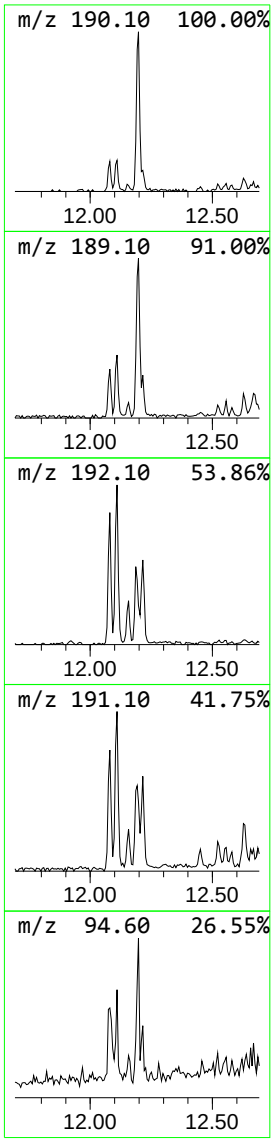
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.192	2.09 ng	87573	Phenanthrene-d10	11.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	47
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	25
4	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	20
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	20





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Misc :
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF051424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

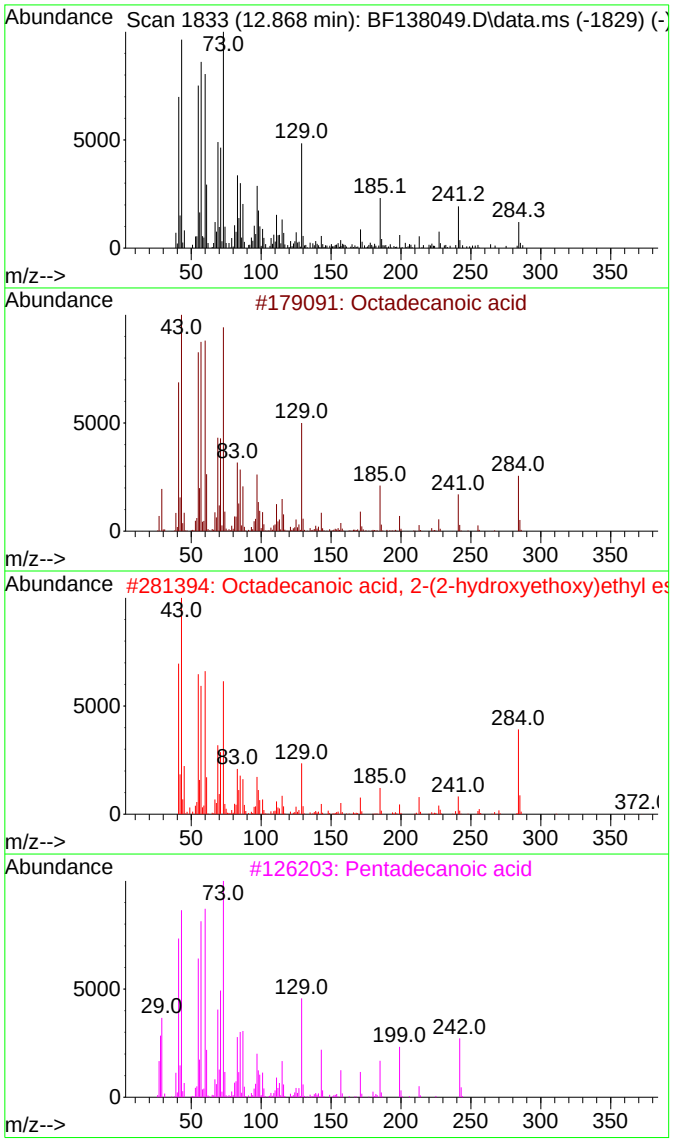
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

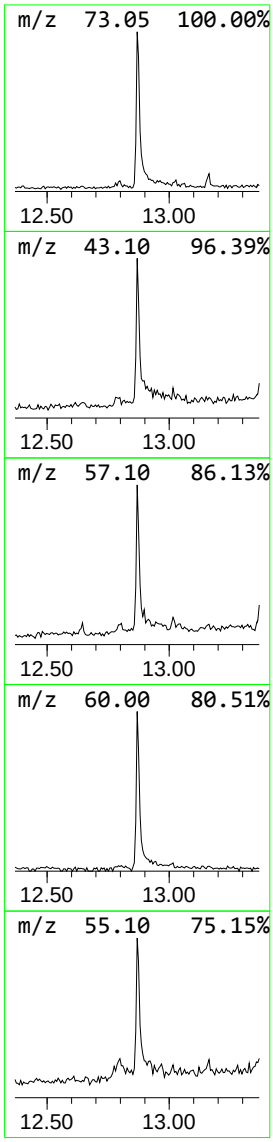
****

Peak Number 6 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.868	5.57 ng	233251	Phenanthrene-d10	11.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF051424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

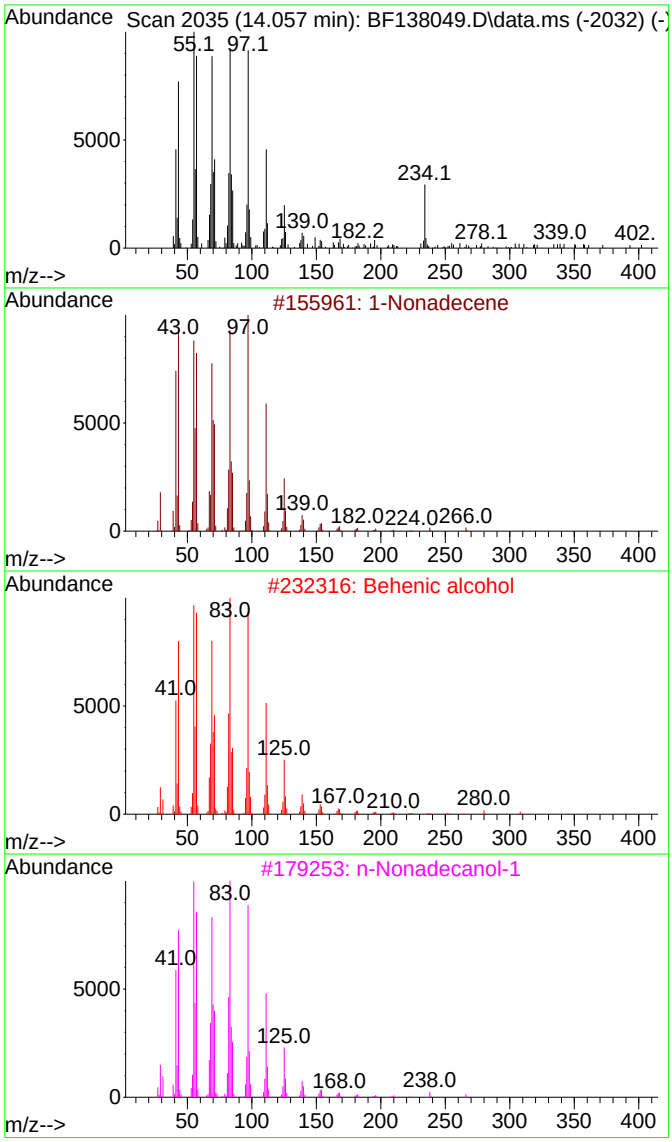
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

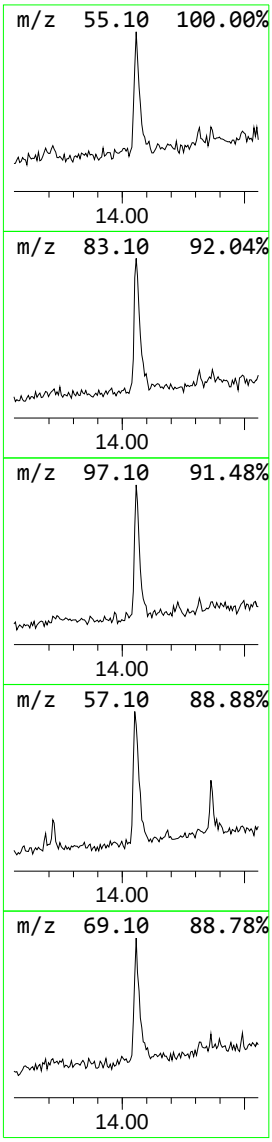
****

Peak Number 7 1-Nonadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.057	5.17 ng	276192	Chrysene-d12	14.227

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	98
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4	1-Heneicosanol	312	C21H44O	015594-90-8	95
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052824\
Data File : BF138049.D
Acq On : 28 May 2024 16:07
Operator : CG\JU
Sample : P2616-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-206

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF051424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

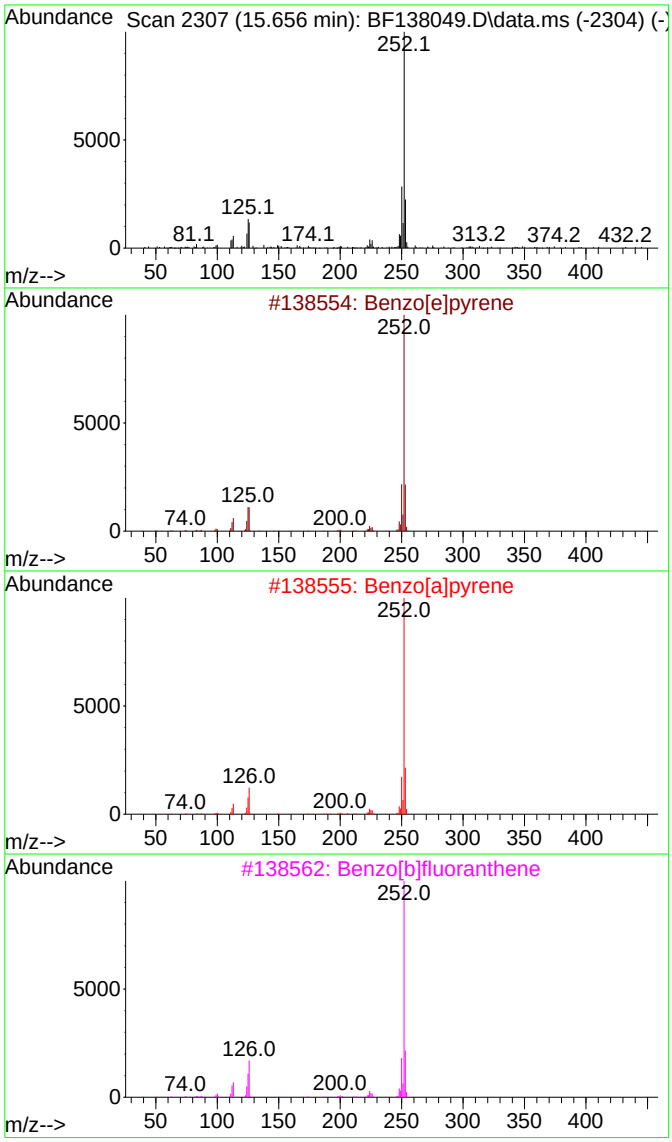
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

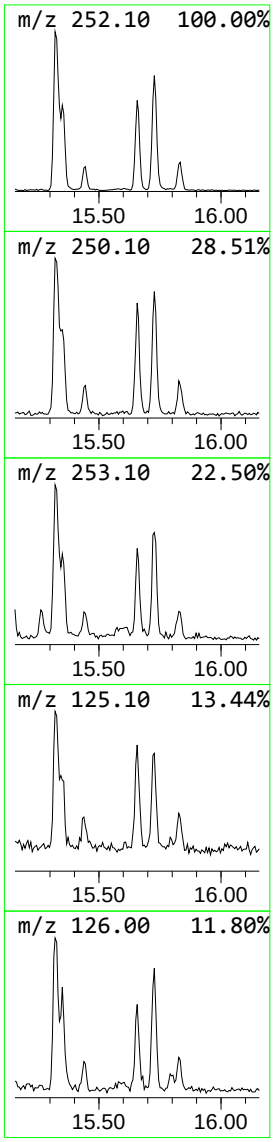
****

Peak Number 8 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.656	4.53 ng	123589	Perylene-d12	15.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[a]pyrene	252	C20H12	000050-32-8	97
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
5	Perylene	252	C20H12	000198-55-0	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052824\
Data File : BF138049.D
Acq On : 28 May 2024 16:07
Operator : CG\JU
Sample : P2616-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-206

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF051424.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...	2.404	39.7	ng	1644900	1	7.033	829022	20.0
Ethanol, 2-(2-b...	8.204	2.6	ng	138123	2	8.316	1050490	20.0
n-Hexadecanoic ...	12.086	9.5	ng	399531	4	11.574	837715	20.0
1H-Cyclopropa[l...	12.110	2.1	ng	89524	4	11.574	837715	20.0
4H-Cyclopenta[d...	12.192	2.1	ng	87573	4	11.574	837715	20.0
Octadecanoic acid	12.868	5.6	ng	233251	4	11.574	837715	20.0
1-Nonadecene	14.057	5.2	ng	276192	5	14.227	1068550	20.0
Benzo[e]pyrene	15.656	4.5	ng	123589	6	15.798	546159	20.0