LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061924\
Data File : BF138254.D
Acq On : 19 Jun 2024 19:28
Operator : CG\JU
Sample : P2955-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-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-BF061224.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138254.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	11	17	22	rVB	3081488	3795649	90.13%	8.892%
2	3.393	218	222	234	rBV	102833	235709	5.60%	0.552%
3	3.481	234	237	251	rVB4	22523	65762	1.56%	0.154%
4	3.975	311	321	332	rBV	54265	86621	2.06%	0.203%
5	5.069	502	507	509	rBV2	38366	56016	1.33%	0.131%
6	5.098	509	512	518	rVB	286424	341742	8.11%	0.801%
7	5.504	568	581	584	rBV	4369956	3946509	93.71%	9.246%
8	5.828	633	636	641	rVB	67269	59537	1.41%	0.139%
9	5.904	641	649	653	rBV4	50955	67852	1.61%	0.159%
10	6.134	683	688	691	rBV3	48125	73385	1.74%	0.172%
11	6.322	715	720	723	rBV2	40151	52660	1.25%	0.123%
12	6.416	733	736	742	rBV4	56120	90403	2.15%	0.212%
13	6.510	747	752	755	rVV	4110720	3738836	88.78%	8.759%
14	6.704	782	785	790	rBV	342203	313098	7.43%	0.734%
15	6.887	812	816	819	rVB	2033205	1808776	42.95%	4.237%
16	6.939	822	825	829	rBV4	66068	69984	1.66%	0.164%
17	7.281	878	883	886	rBV3	73971	84452	2.01%	0.198%
18	7.445	906	911	914	rBV	2894015	2464564	58.52%	5.774%
19	7.475	914	916	920	rVB	95808	82728	1.96%	0.194%
20	7.522	920	924	928	rVB4	47228	67148	1.59%	0.157%
21	7.581	928	934	938	rBV5	37972	73159	1.74%	0.171%
22	7.692	950	953	957	rVB2	190324	168984	4.01%	0.396%
23	8.104	1020	1023	1027	rBV4	53913	65644	1.56%	0.154%
24	8.163	1030	1033	1036	rVV	2737607	2252743	53.49%	5.278%
25	8.186	1036	1037	1040	rVV	162437	97278	2.31%	0.228%
26	8.222	1040	1043	1046	rVB2	111081	97690	2.32%	0.229%
27	8.381	1065	1070	1073	rBV	77314	61896	1.47%	0.145%
28	8.475	1076	1086	1090	rBV	480878	512513	12.17%	1.201%
29	8.586	1101	1105	1107	rBV	135098	130859	3.11%	0.307%
30	8.751	1130	1133	1137	rBV	147423	116337	2.76%	0.273%
31	8.875	1152	1154	1157	rVB	118915	83636	1.99%	0.196%
32	8.975	1168	1171	1174	rBV	84810	67254	1.60%	0.158%
33	9.157	1199	1202	1204	rBV2	68734	55929	1.33%	0.131%
34	9.180	1204	1206	1212	rVB	77190	70074	1.66%	0.164%
35	9.239	1212	1216	1219	rBV	5352593	4211501	100.00%	9.866%
36	9.316	1226	1229	1232	rBV	369483	348216	8.27%	0.816%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061924\
Data File : BF138254.D
Acq On : 19 Jun 2024 19:28
Operator : CG\JU
Sample : P2955-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-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-BF061224.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	9.498	1257	1260	1265	rBV6	56075	86446	2.05%	0.203%
38	9.575	1270	1273	1275	rVB2	87046	71686	1.70%	0.168%
39	9.598	1275	1277	1279	rVB2	61606	52210	1.24%	0.122%
40	9.628	1279	1282	1286	rBV2	211802	239886	5.70%	0.562%
41	9.692	1289	1293	1295	rBV4	64010	75734	1.80%	0.177%
42	9.733	1298	1300	1303	rVB3	80981	67598	1.61%	0.158%
43	9.786	1306	1309	1311	rBV3	176052	181030	4.30%	0.424%
44	9.810	1311	1313	1314	rBV	85830	58315	1.38%	0.137%
45	9.828	1314	1316	1318	rBV	168828	123856	2.94%	0.290%
46	9.916	1325	1331	1335	rBV	2236799	2115294	50.23%	4.956%
47	9.957	1335	1338	1342	rBV4	76462	121395	2.88%	0.284%
48	10.016	1343	1348	1353	rVV	1677330	2284628	54.25%	5.352%
49	10.233	1383	1385	1387	rBV2	65496	62764	1.49%	0.147%
50	10.257	1387	1389	1392	rVB3	141068	118563	2.82%	0.278%
51	10.327	1398	1401	1403	rBV2	166620	143702	3.41%	0.337%
52	10.380	1407	1410	1412	rBV3	76437	98404	2.34%	0.231%
53	10.457	1421	1423	1426	rBV3	87977	110197	2.62%	0.258%
54	10.704	1461	1465	1468	rBV	2272131	1900054	45.12%	4.451%
55	10.833	1483	1487	1490	rBV2	285164	315980	7.50%	0.740%
56	11.069	1524	1527	1530	rBV4	118401	137380	3.26%	0.322%
57	11.404	1581	1584	1587	rBV	2117343	1674630	39.76%	3.923%
58	11.427	1587	1588	1594	rVB	225992	181033	4.30%	0.424%
59	11.933	1671	1674	1683	rVB2	748714	848340	20.14%	1.987%
60	12.716	1805	1807	1810	rBV3	339903	323559	7.68%	0.758%
61	12.992	1850	1854	1857	rBV	3570469	3199388	75.97%	7.495%
62	14.045	2030	2033	2036	rBV	1476321	1275224	30.28%	2.988%
63	15.521	2281	2284	2287	rVB	826106	902605	21.43%	2.115%

Sum of corrected areas: 42685045

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061924\
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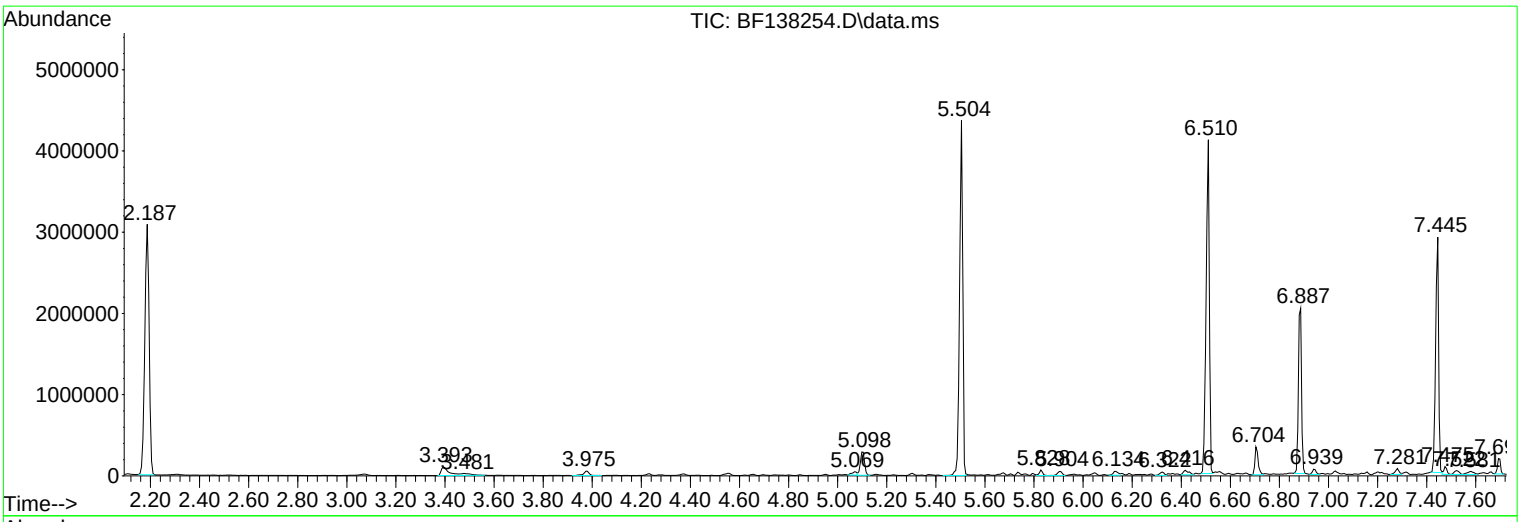
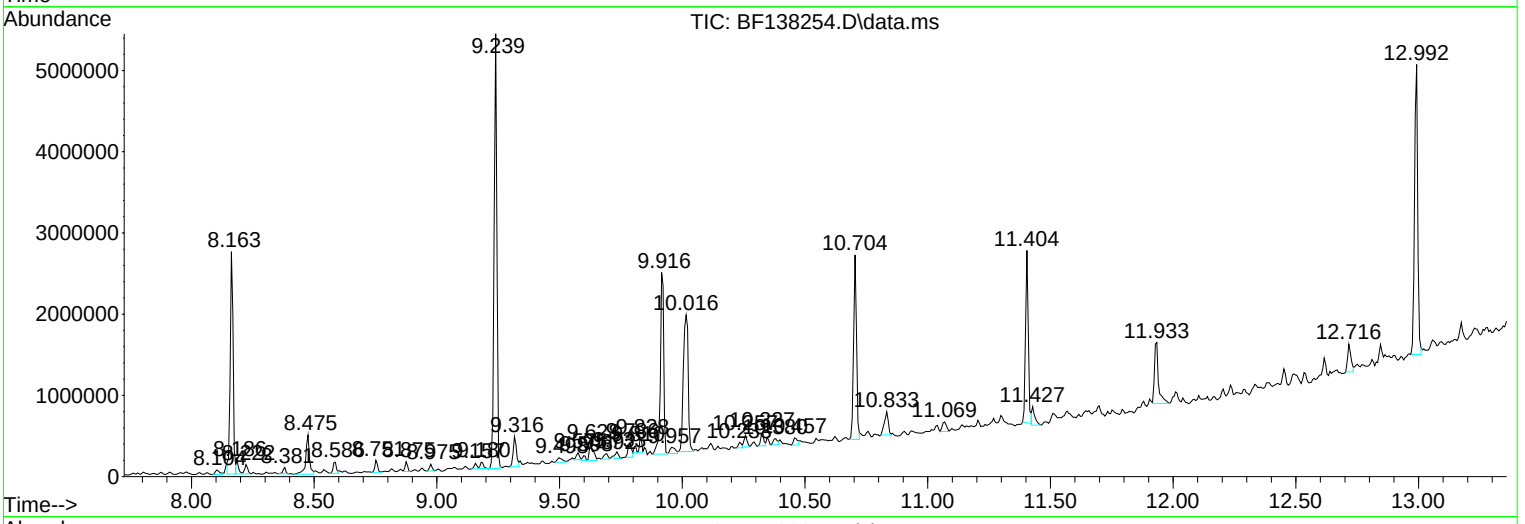
Misc :
ALS Vial : 11 Sample Multiplier: 1

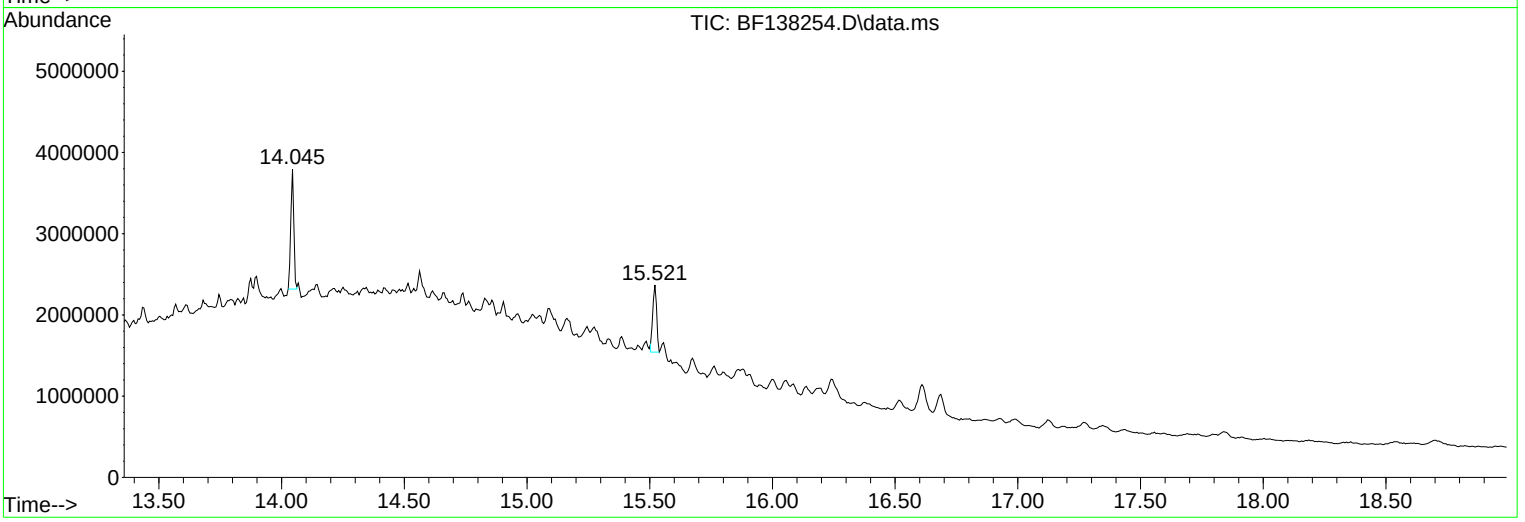
Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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\BF061924\
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Operator : CG\JU
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BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

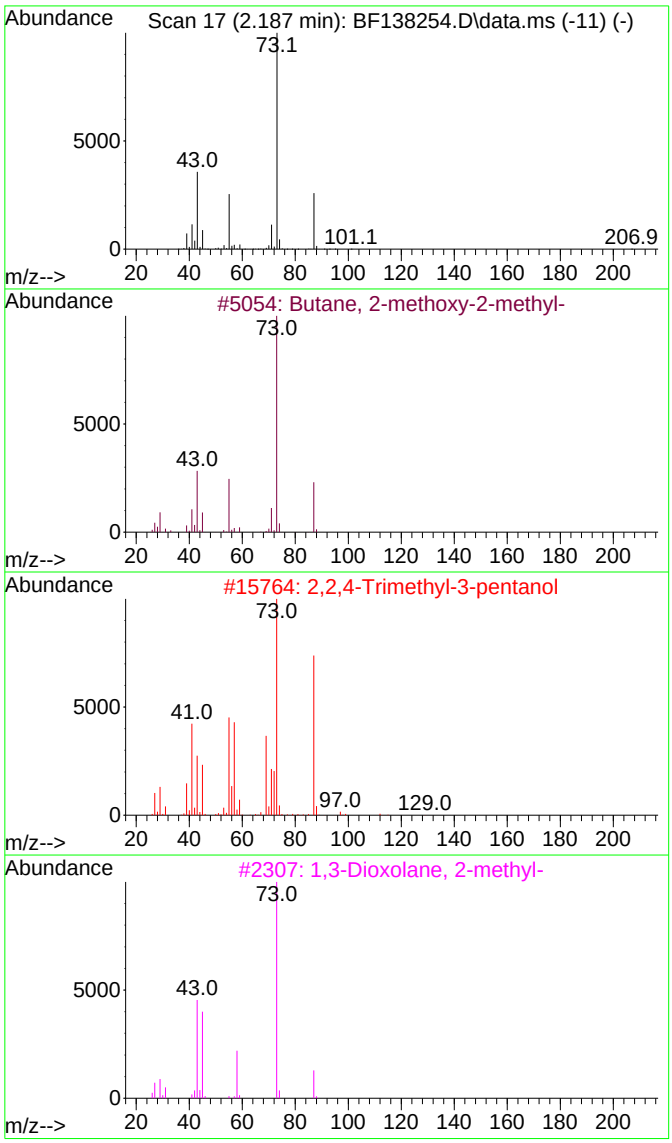
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

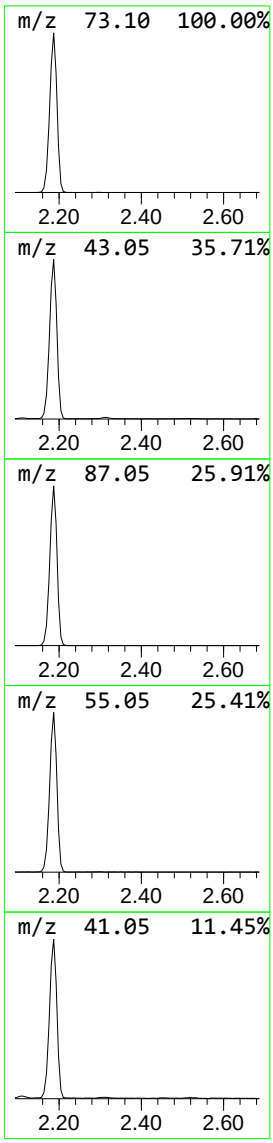
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.187	41.97 ng	3795650	1,4-Dichlorobenzene-d4	6.887

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061924\
Data File : BF138254.D
Acq On : 19 Jun 2024 19:28
Operator : CG\JU
Sample : P2955-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

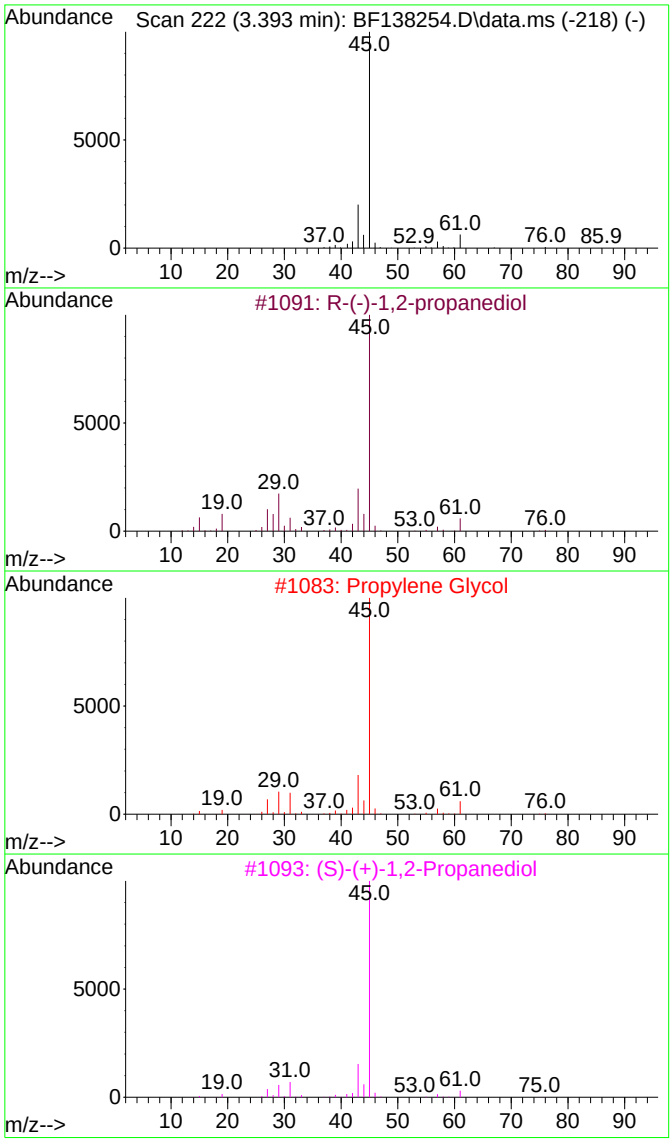
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

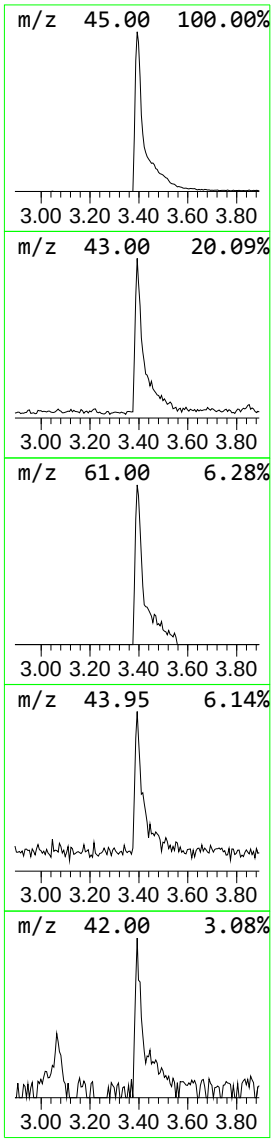
****

Peak Number 2 R-(-)-1,2-propanediol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.393	2.61 ng	235709	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	83
2	Propylene Glycol	76	C3H8O2	000057-55-6	78
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5	Isopropyl Alcohol	60	C3H8O	000067-63-0	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061924\
Data File : BF138254.D
Acq On : 19 Jun 2024 19:28
Operator : CG\JU
Sample : P2955-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

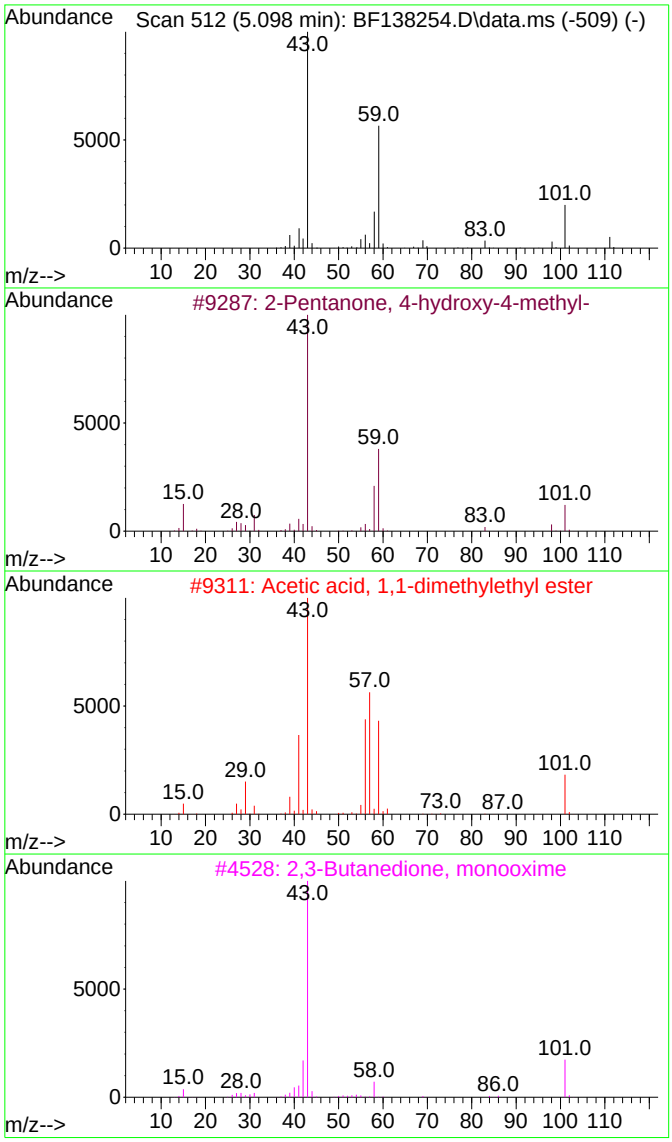
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

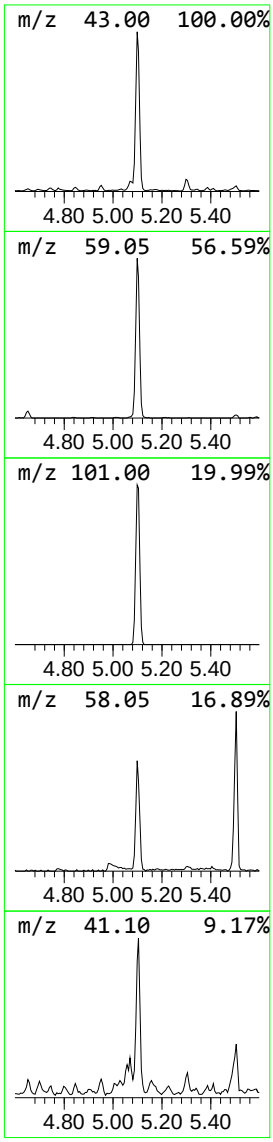
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	3.78 ng	341742	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	2-Decanol, methyl ether	172	C11H24O	1000333-83-9	23
5	Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061924\
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Sample : P2955-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

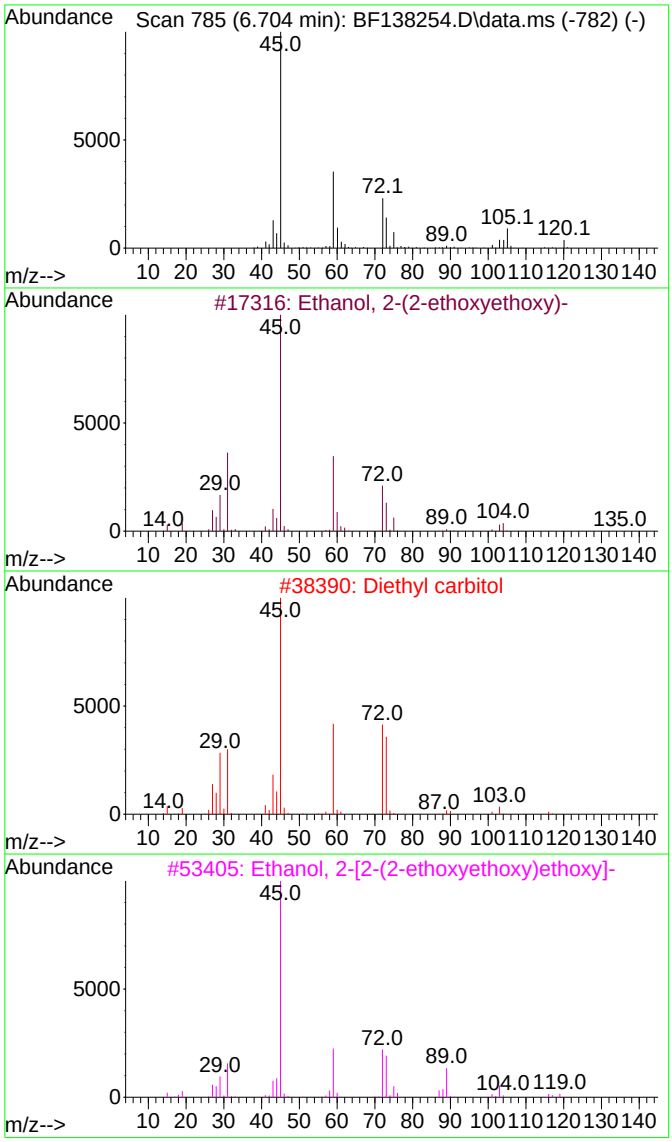
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

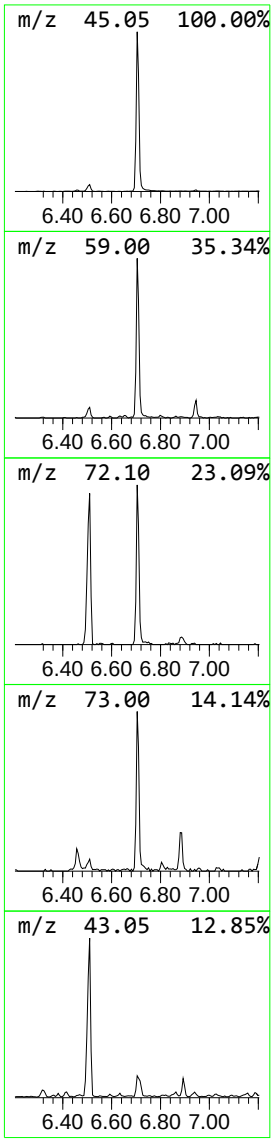
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.704	3.46 ng	313098	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	86
2	Diethyl carbitol	162	C8H18O3	000112-36-7	64
3	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	59
4	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	42
5	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061924\
Data File : BF138254.D
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Sample : P2955-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

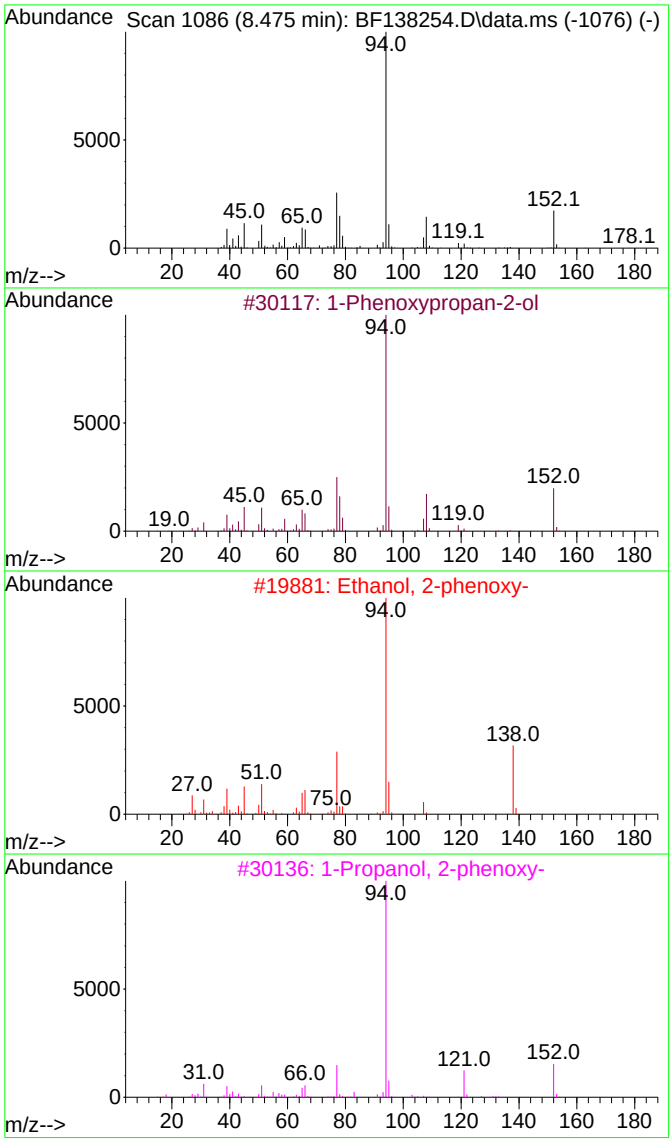
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

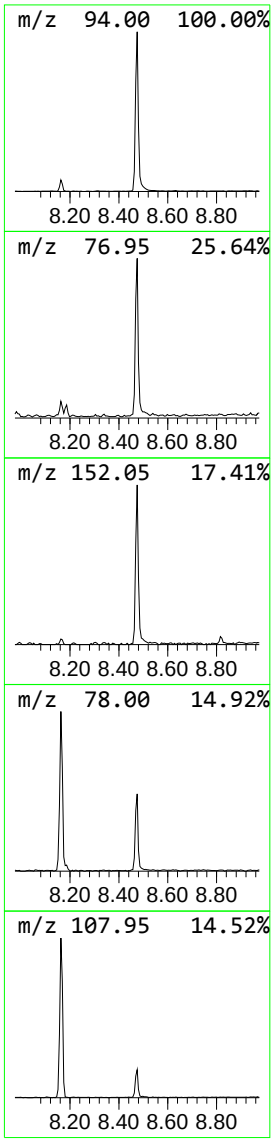
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.475	4.55 ng	512513	Naphthalene-d8	8.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
3	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
4	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	60
5	Benzene, propoxy-	136	C9H12O	000622-85-5	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061924\
Data File : BF138254.D
Acq On : 19 Jun 2024 19:28
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Sample : P2955-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

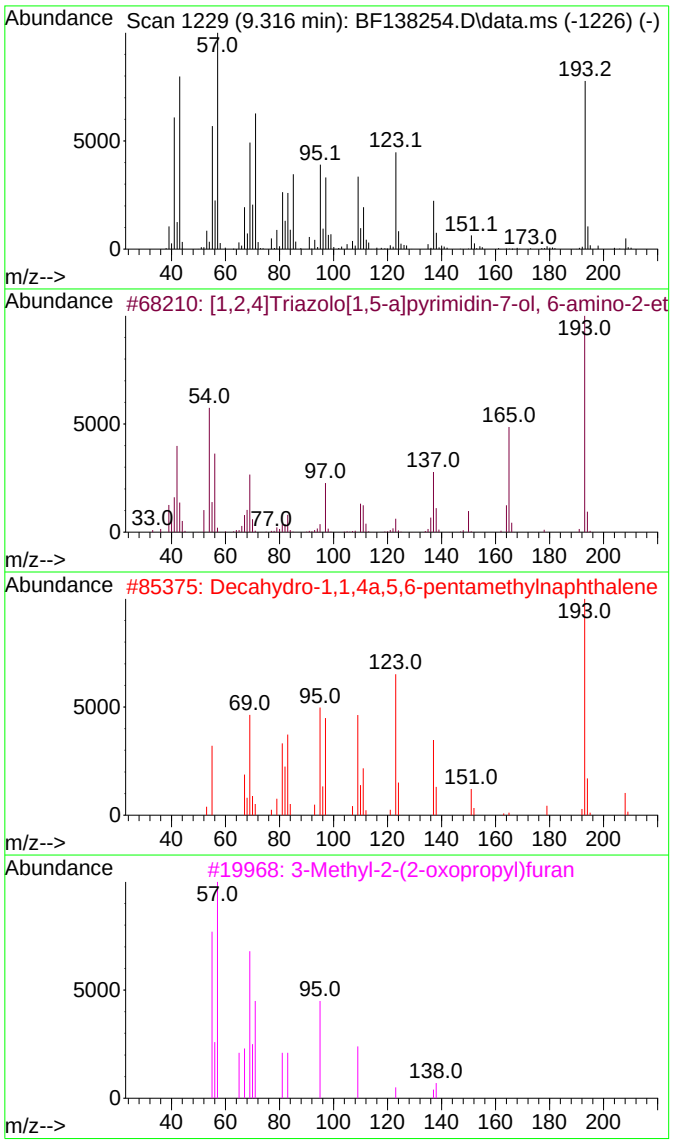
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

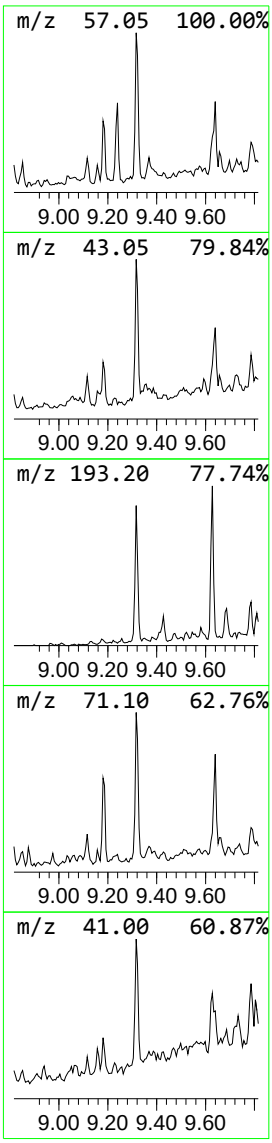
****

Peak Number 6 unknown9.316 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.316	3.29 ng	348216	Acenaphthene-d10	9.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	[1,2,4]Triazolo[1,5-a]pyrimidin-...	193	C8H11N5O	1000351-50-1	30
2	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	30
3	3-Methyl-2-(2-oxopropyl)furan	138	C8H10O2	087773-62-4	15
4	Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	15
5	2,6,10-Trimethylundeca-1,3-diene	194	C14H26	1000222-09-1	15





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061924\
Data File : BF138254.D
Acq On : 19 Jun 2024 19:28
Operator : CG\JU
Sample : P2955-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

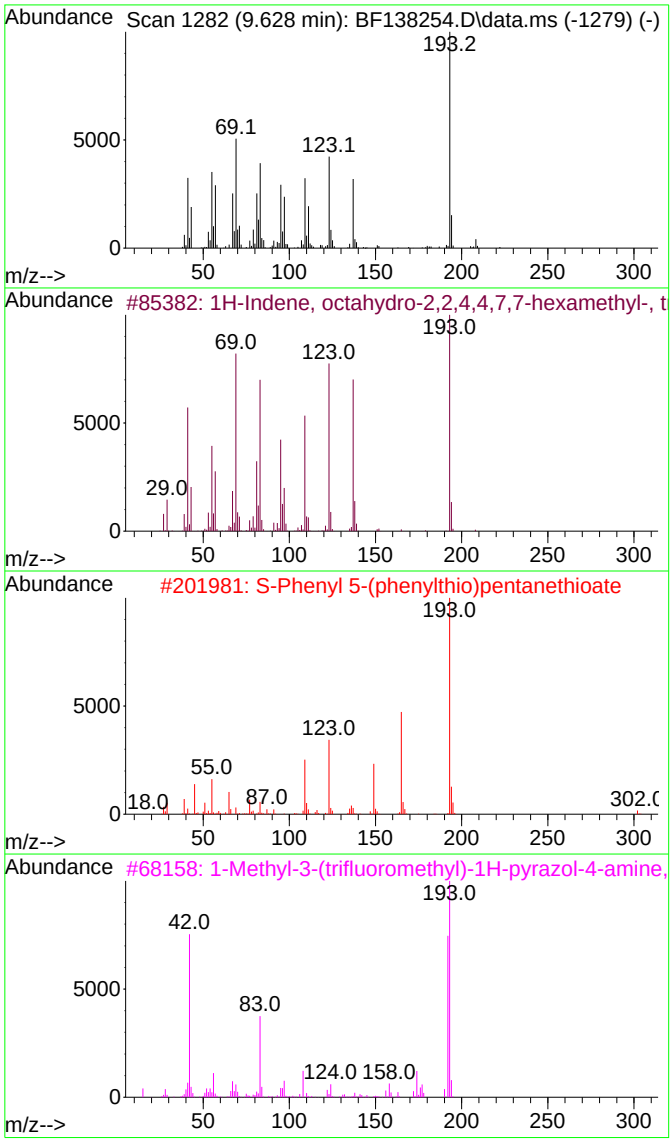
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

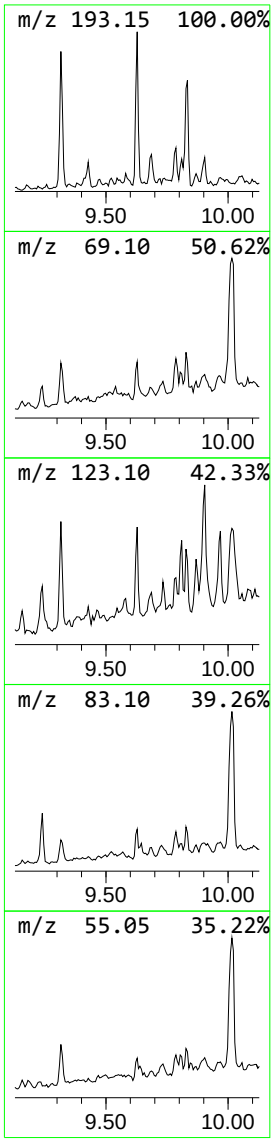
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1H-Indene, octahydro-2,2,4,... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.628	2.27 ng	239886	Acenaphthene-d10	9.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	53
2	S-Phenyl 5-(phenylthio)pentaneth...	302	C17H18OS2	1000234-40-7	43
3	1-Methyl-3-(trifluoromethyl)-1H-...	193	C7H10F3N3	1000511-73-1	38
4	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	38
5	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061924\
Data File : BF138254.D
Acq On : 19 Jun 2024 19:28
Operator : CG\JU
Sample : P2955-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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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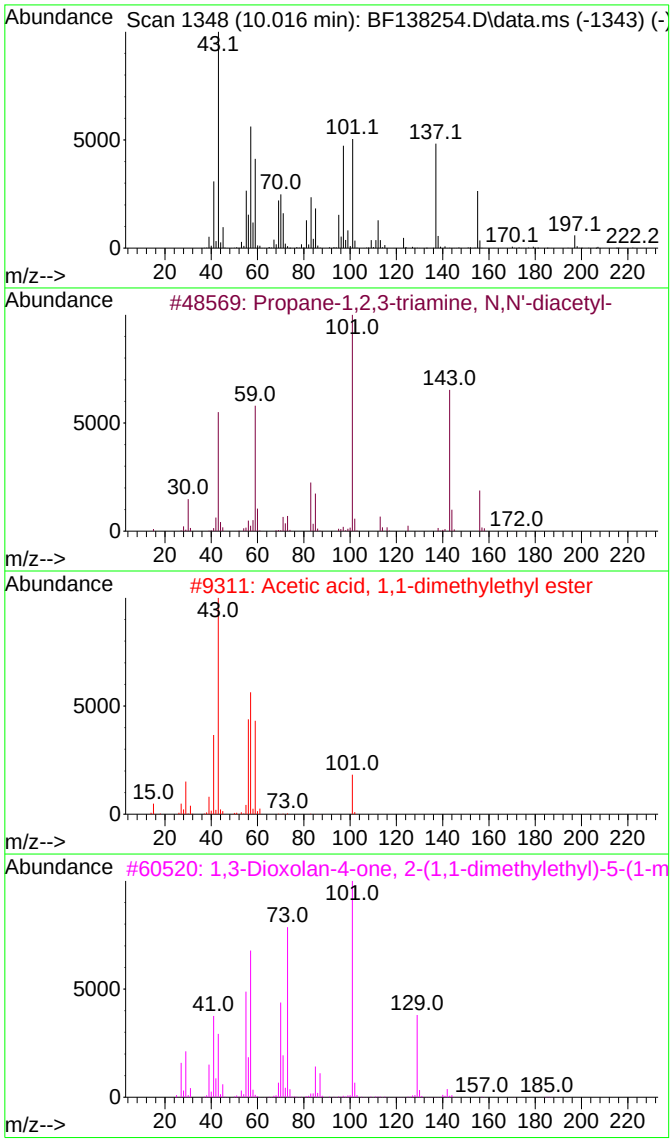
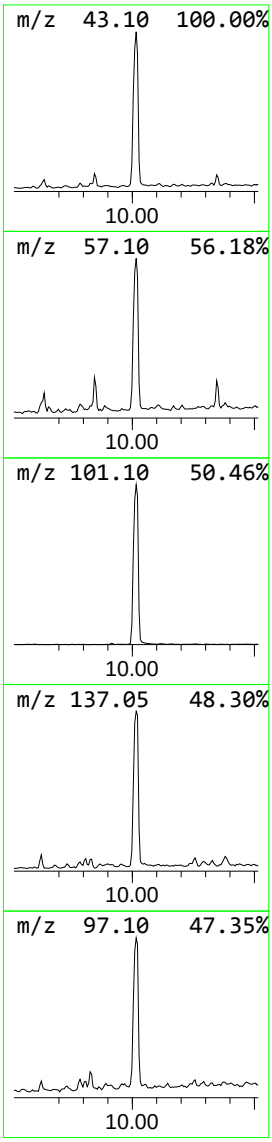
Peak Number 8 unknown10.016 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.016	21.60 ng	2284630	Acenaphthene-d10	9.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane-1,2,3-triamine, N,N'-dia...	173	C7H15N3O2	1000500-54-4	16
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	12
3	1,3-Dioxolan-4-one, 2-(1,1-dimet...	186	C10H18O3	089053-56-5	11
4	Succinic acid, cyclohexyl hexyl ...	284	C16H28O4	1010330-01-7	10
5	Butane, 1,1'-[methylenebis(oxy)]...	188	C11H24O2	022418-64-0	10





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Sample : P2955-05
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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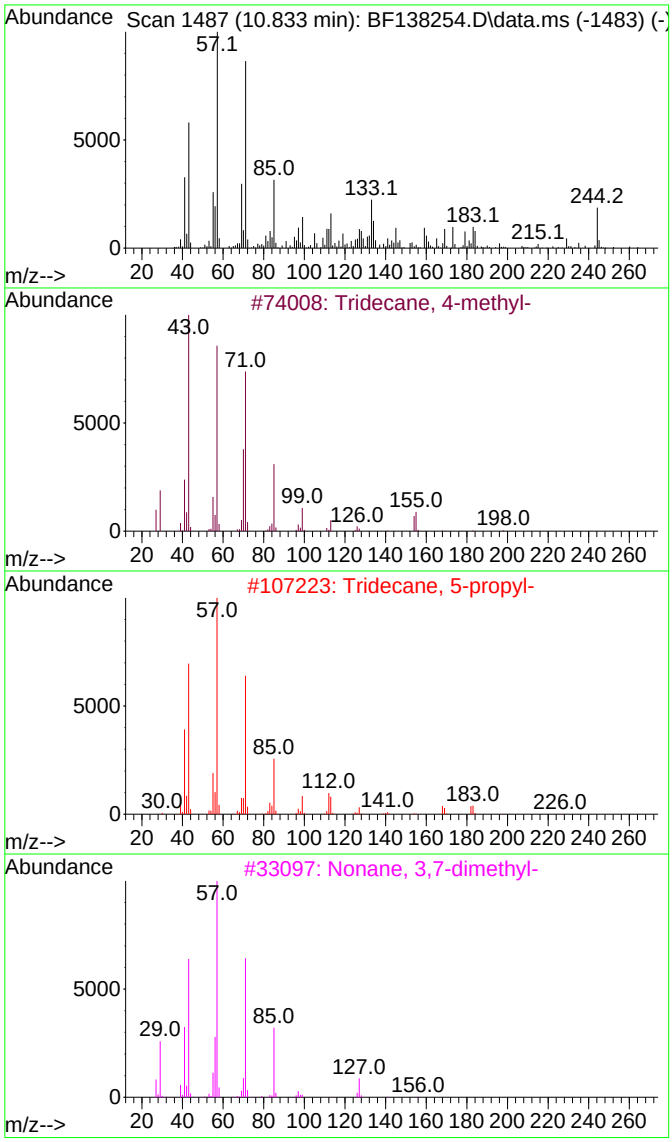
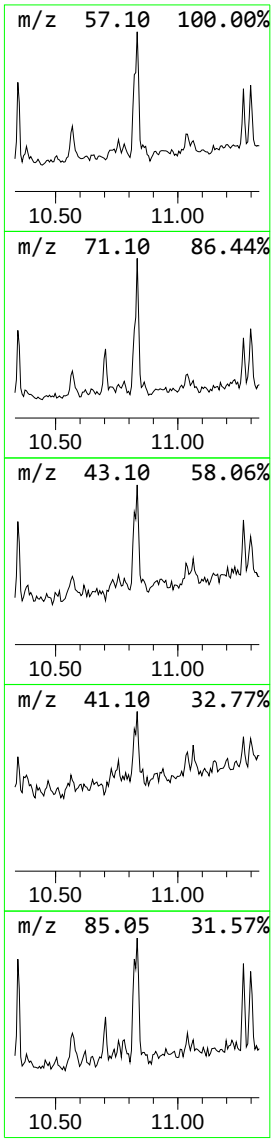
Peak Number 9 unknown10.833 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.833	3.77 ng	315980	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 4-methyl-	198	C14H30	026730-12-1	49
2	Tridecane, 5-propyl-	226	C16H34	055045-11-9	49
3	Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	49
4	Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	46
5	Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1010309-19-2	43





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Data File : BF138254.D
Acq On : 19 Jun 2024 19:28
Operator : CG\JU
Sample : P2955-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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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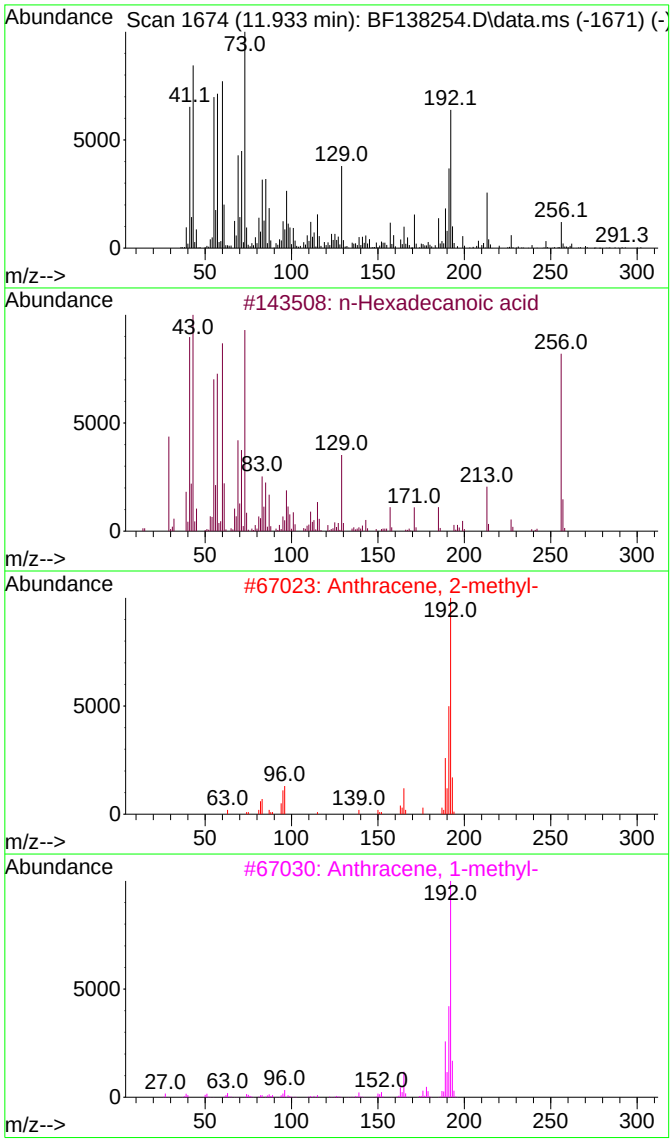
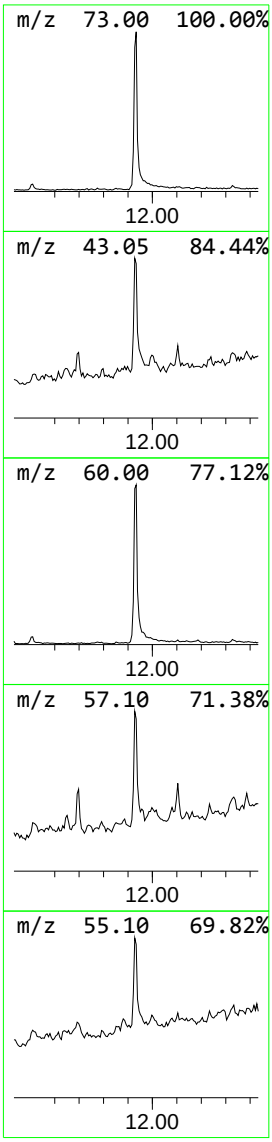
Peak Number 10 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	10.13 ng	848340	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	90
4	Tridecanoic acid	214	C13H26O2	000638-53-9	78
5	Octadecanoic acid	284	C18H36O2	000057-11-4	70





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Sample : P2955-05
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BNA_F
ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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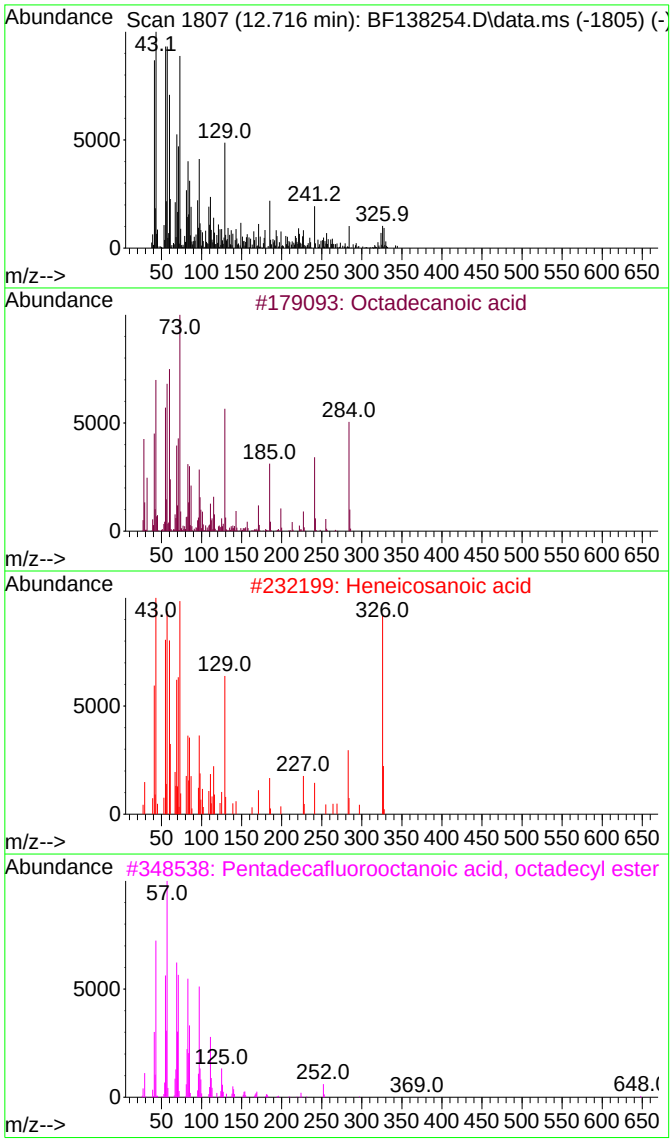
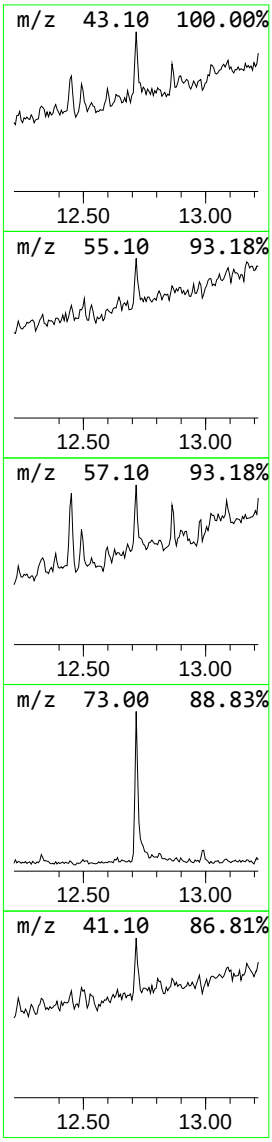
Peak Number 11 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	3.86 ng	323559	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Heneicosanoic acid	326	C21H42O2	002363-71-5	89
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	43
4	1-Octadecene	252	C18H36	000112-88-9	42
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	42





Tentatively Identified Compound (LSC) summary

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Data File : BF138254.D
Acq On : 19 Jun 2024 19:28
Operator : CG\JU
Sample : P2955-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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...	2.187	42.0	ng	3795650	1	6.887	1808780	20.0
R-(-)-1,2-propa...	3.393	2.6	ng	235709	1	6.887	1808780	20.0
2-Pentanone, 4-...	5.098	3.8	ng	341742	1	6.887	1808780	20.0
Ethanol, 2-(2-e...	6.704	3.5	ng	313098	1	6.887	1808780	20.0
1-Phenoxypropan...	8.475	4.5	ng	512513	2	8.163	2252740	20.0
unknown9.316	9.316	3.3	ng	348216	3	9.916	2115290	20.0
1H-Indene, octa...	9.628	2.3	ng	239886	3	9.916	2115290	20.0
unknown10.016	10.016	21.6	ng	2284630	3	9.916	2115290	20.0
unknown10.833	10.833	3.8	ng	315980	4	11.404	1674630	20.0
n-Hexadecanoic ...	11.933	10.1	ng	848340	4	11.404	1674630	20.0
Octadecanoic acid	12.716	3.9	ng	323559	4	11.404	1674630	20.0