LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061021\
Data File : BF124245.D
Acq On : 10 Jun 2021 22:01
Operator : JU/CG
Sample : M2651-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 17-B6(4-8)

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-BF060321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124245.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	14	18	24	rBB3	13562	19875	1.89%	0.237%
2	5.057	502	505	514	rVB	60129	74286	7.06%	0.885%
3	5.475	572	576	587	rBV	909921	872567	82.89%	10.391%
4	6.493	744	749	752	rBV	1025748	903849	85.86%	10.764%
5	6.675	777	780	786	rBB2	31904	30607	2.91%	0.364%
6	6.845	806	809	813	rVB	311173	228660	21.72%	2.723%
7	7.410	900	905	908	rBV	704167	606749	57.64%	7.226%
8	8.128	1024	1027	1031	rBV	363727	289252	27.48%	3.445%
9	9.204	1206	1210	1213	rBV	1299461	1052736	100.00%	12.537%
10	9.334	1225	1232	1236	rBV3	22057	30501	2.90%	0.363%
11	9.598	1273	1277	1280	rBV	263621	191938	18.23%	2.286%
12	9.886	1322	1326	1329	rBV	460655	356619	33.88%	4.247%
13	10.675	1456	1460	1464	rBV	943025	810309	76.97%	9.650%
14	11.375	1575	1579	1581	rBV	393160	347472	33.01%	4.138%
15	11.392	1581	1582	1585	rVB	19479	12892	1.22%	0.154%
16	11.898	1665	1668	1672	rBV	127835	112038	10.64%	1.334%
17	12.586	1782	1785	1789	rBV	44512	42962	4.08%	0.512%
18	12.680	1798	1801	1805	rBV3	31362	30632	2.91%	0.365%
19	12.774	1813	1817	1820	rBV2	19484	18964	1.80%	0.226%
20	12.816	1820	1824	1828	rVB	38792	39267	3.73%	0.468%
21	12.957	1844	1848	1851	rVB	1161339	941414	89.43%	11.211%
22	13.139	1874	1879	1882	rVB4	7929	12762	1.21%	0.152%
23	13.186	1882	1887	1889	rBV2	10503	16341	1.55%	0.195%
24	13.433	1922	1929	1936	rBV	264310	275521	26.17%	3.281%
25	13.857	1997	2001	2011	rBV3	83036	150743	14.32%	1.795%
26	14.016	2020	2028	2031	rBV	309717	301632	28.65%	3.592%
27	14.039	2031	2032	2035	rVB	25390	15704	1.49%	0.187%
28	14.174	2051	2055	2056	rBV4	15696	16354	1.55%	0.195%
29	14.474	2103	2106	2108	rBV2	18604	20347	1.93%	0.242%
30	15.057	2202	2205	2214	rVB3	31427	50930	4.84%	0.607%
31	15.121	2214	2216	2221	rVB5	18022	19872	1.89%	0.237%
32	15.163	2221	2223	2226	rBV3	16439	17602	1.67%	0.210%
33	15.368	2255	2258	2260	rVB4	11914	13350	1.27%	0.159%
34	15.427	2264	2268	2274	rVB4	22862	31915	3.03%	0.380%
35	15.492	2274	2279	2287	rBV	221734	287725	27.33%	3.426%
36	15.710	2313	2316	2322	rVB7	19994	27662	2.63%	0.329%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061021\
Data File : BF124245.D
Acq On : 10 Jun 2021 22:01
Operator : JU/CG
Sample : M2651-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 17-B6(4-8)

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-BF060321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.945	2353	2356	2363	rVB5	24375	30993	2.94%	0.369%
38	16.010	2363	2367	2368	rBV4	20053	18315	1.74%	0.218%
39	16.062	2374	2376	2381	rVB6	14955	16689	1.59%	0.199%
40	16.739	2487	2491	2493	rBV5	13214	18182	1.73%	0.217%
41	16.974	2525	2531	2532	rBV4	16713	22037	2.09%	0.262%
42	17.045	2539	2543	2549	rVB8	14161	18849	1.79%	0.224%

Sum of corrected areas: 8397114

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061021\
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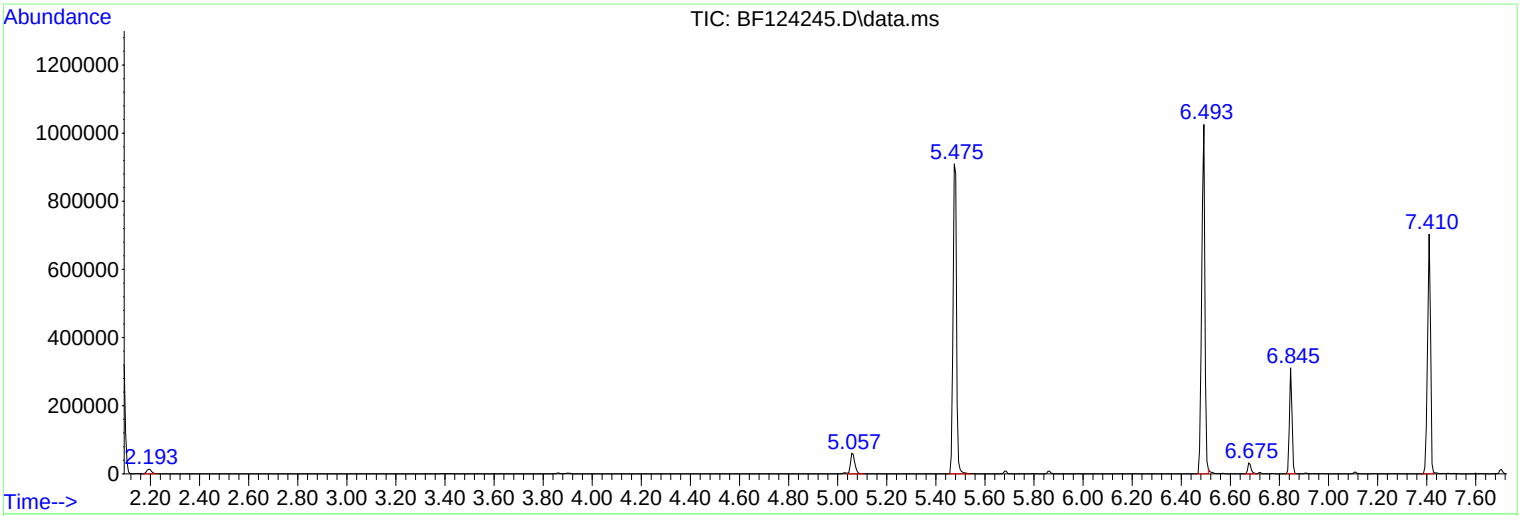
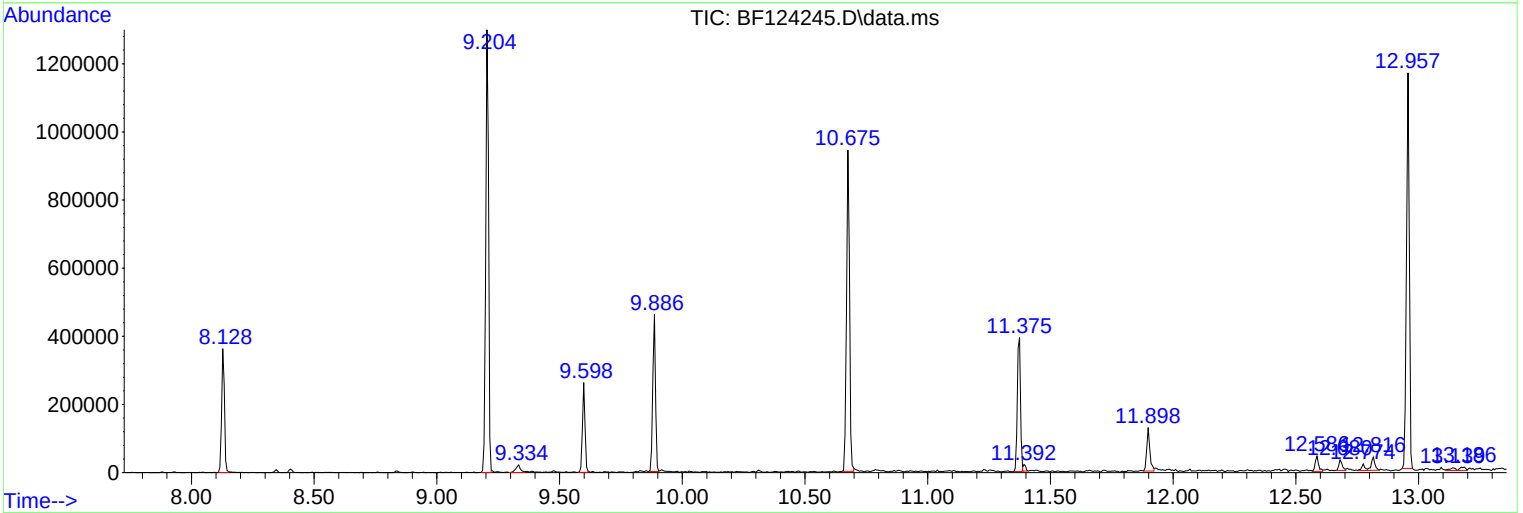
Sample : M2651-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

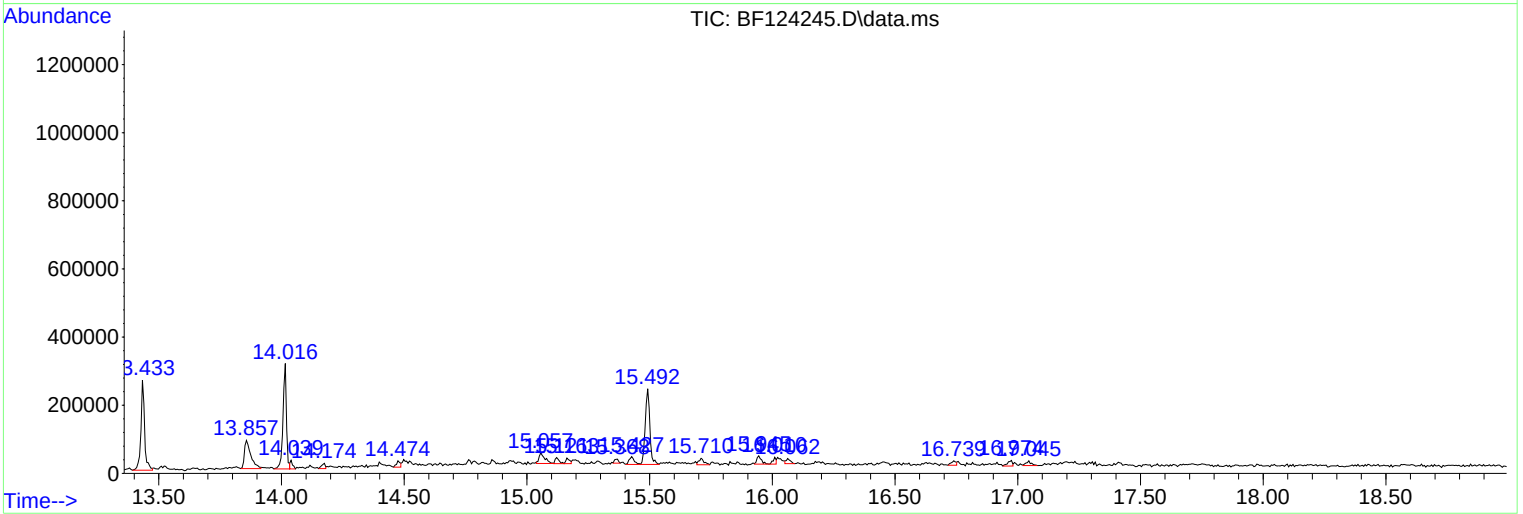
Instrument :
BNA_F
ClientSampleId :
17-B6(4-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061021\
Data File : BF124245.D
Acq On : 10 Jun 2021 22:01
Operator : JU/CG
Sample : M2651-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 17-B6(4-8)

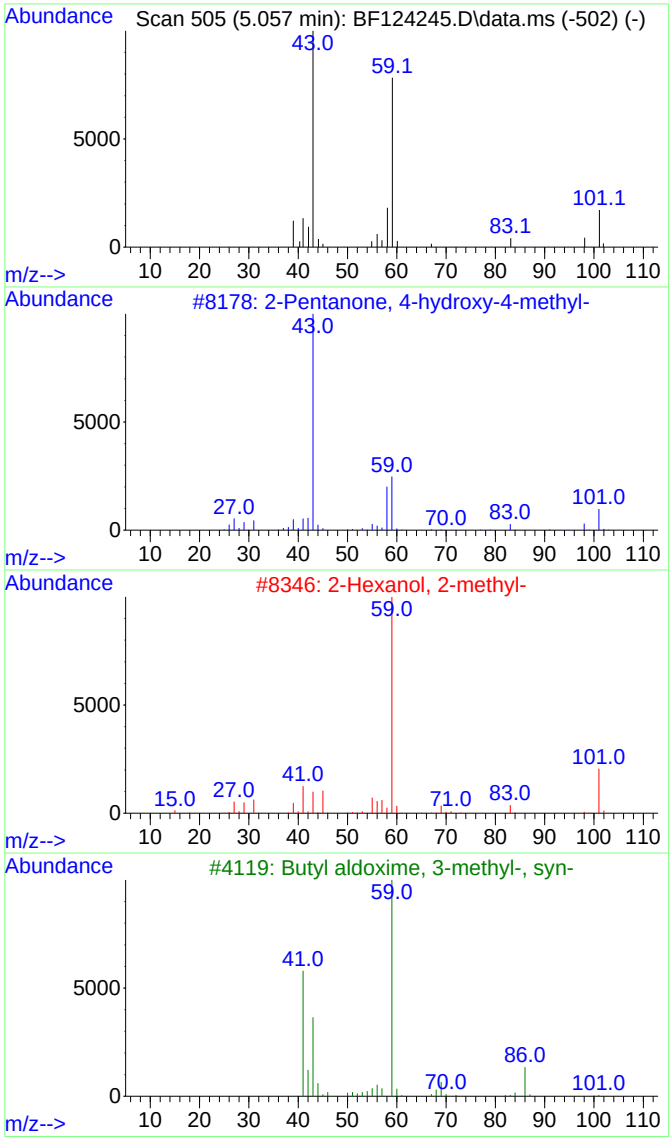
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

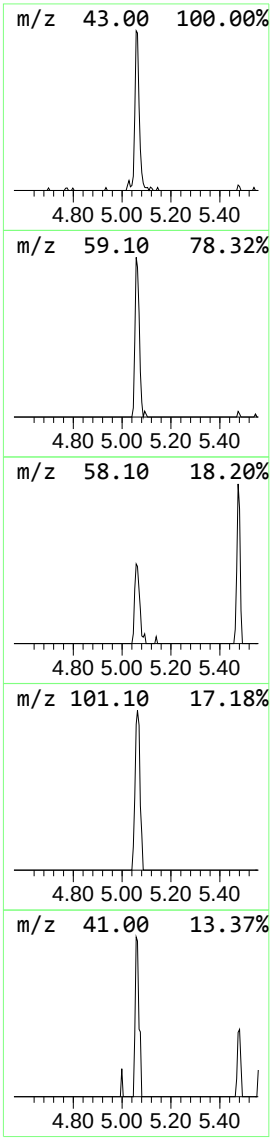
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	6.50 ng	74286	1,4-Dichlorobenzene-d4	6.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	42
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	40
4	2-Hexanone, 3-hydroxy-3,5-dimethyl-	144	C8H16O2	006321-14-8	39
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061021\
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Operator : JU/CG
Sample : M2651-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 17-B6(4-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

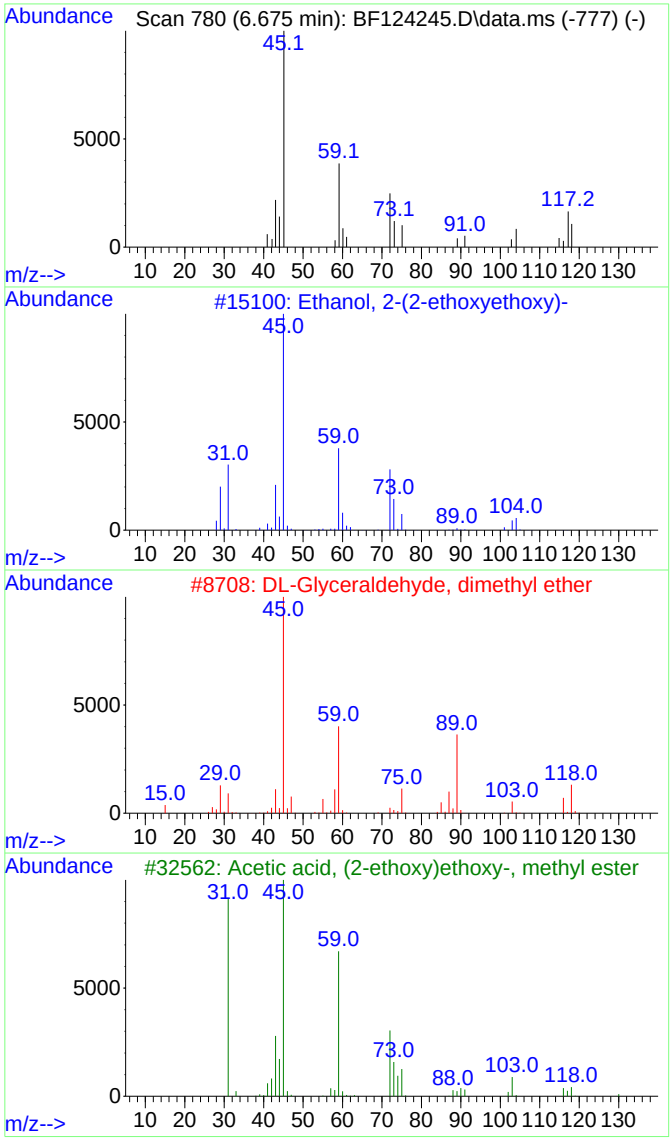
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

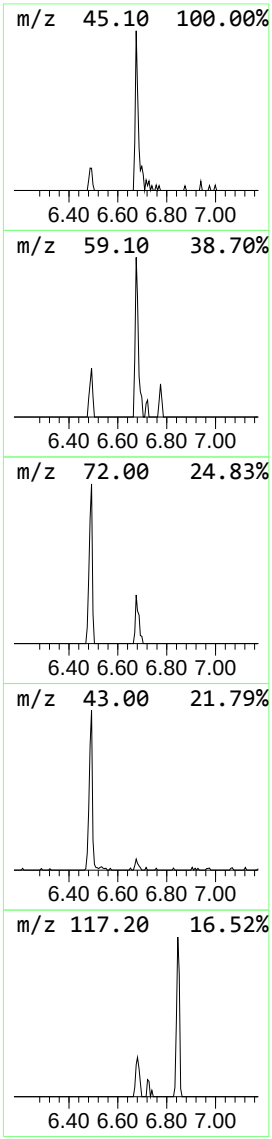
****

Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.675	2.68 ng	30607	1,4-Dichlorobenzene-d4	6.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	72
2	DL-Glyceraldehyde, dimethyl ether	118	C5H10O3	1000332-93-3	59
3	Acetic acid, (2-ethoxy)ethoxy-, ...	162	C7H14O4	016326-34-4	40
4	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	36
5	Tetraethylene glycol diethyl ether	250	C12H26O5	004353-28-0	36





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061021\
Data File : BF124245.D
Acq On : 10 Jun 2021 22:01
Operator : JU/CG
Sample : M2651-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 17-B6(4-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

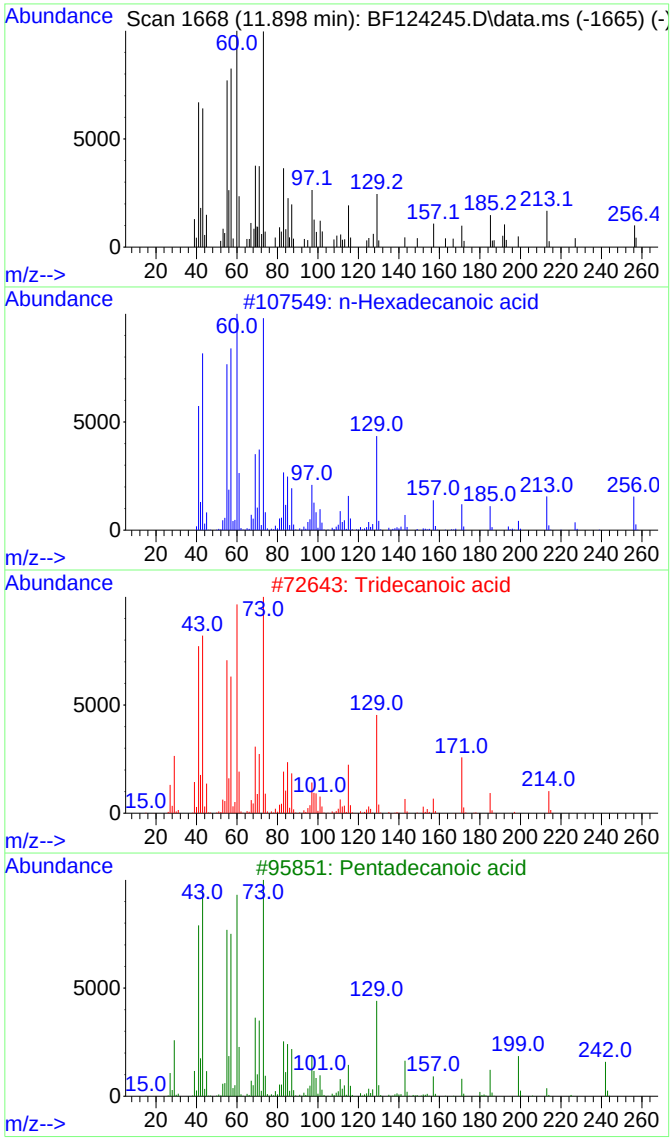
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

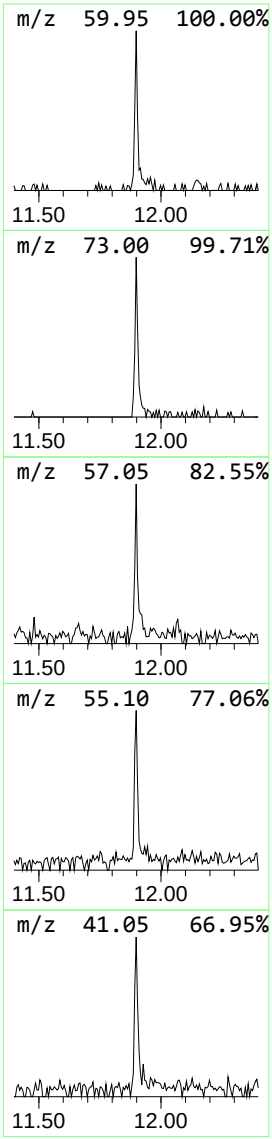
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	6.45 ng	112038	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061021\
Data File : BF124245.D
Acq On : 10 Jun 2021 22:01
Operator : JU/CG
Sample : M2651-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 17-B6(4-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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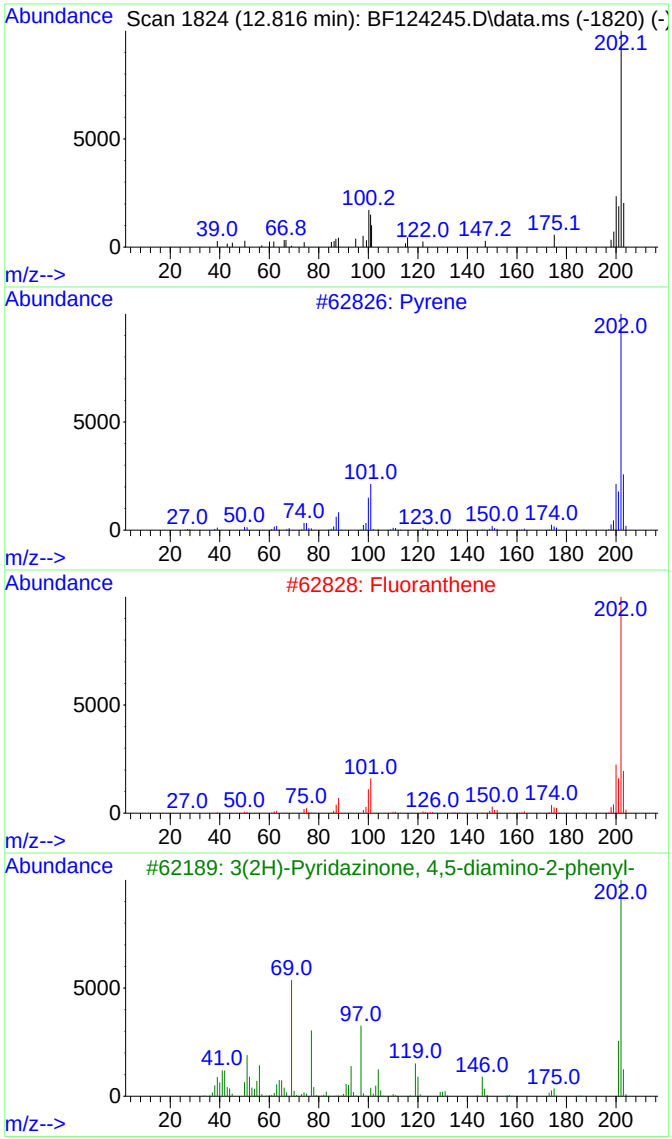
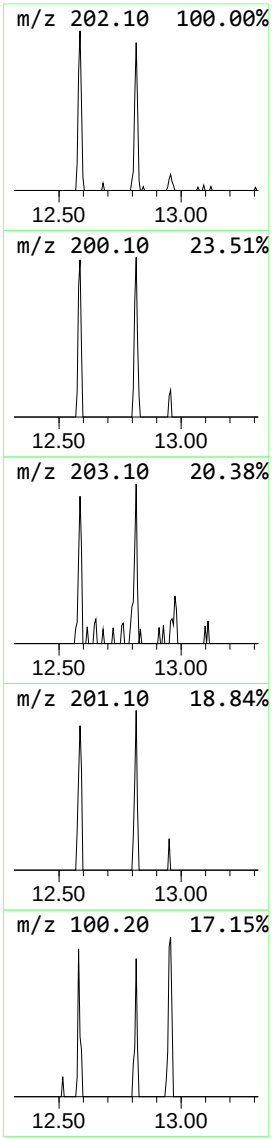
Peak Number 5 unknown12.816 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.816	2.60 ng	39267	Chrysene-d12	14.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene	202	C16H10	000129-00-0	87
2	Fluoranthene	202	C16H10	000206-44-0	72
3	3(2H)-Pyridazinone, 4,5-diamino-...	202	C10H10N4O	1000351-65-9	47
4	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	40
5	Phenol, 4,4'-oxybis-	202	C12H10O3	001965-09-9	7





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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
17-B6(4-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

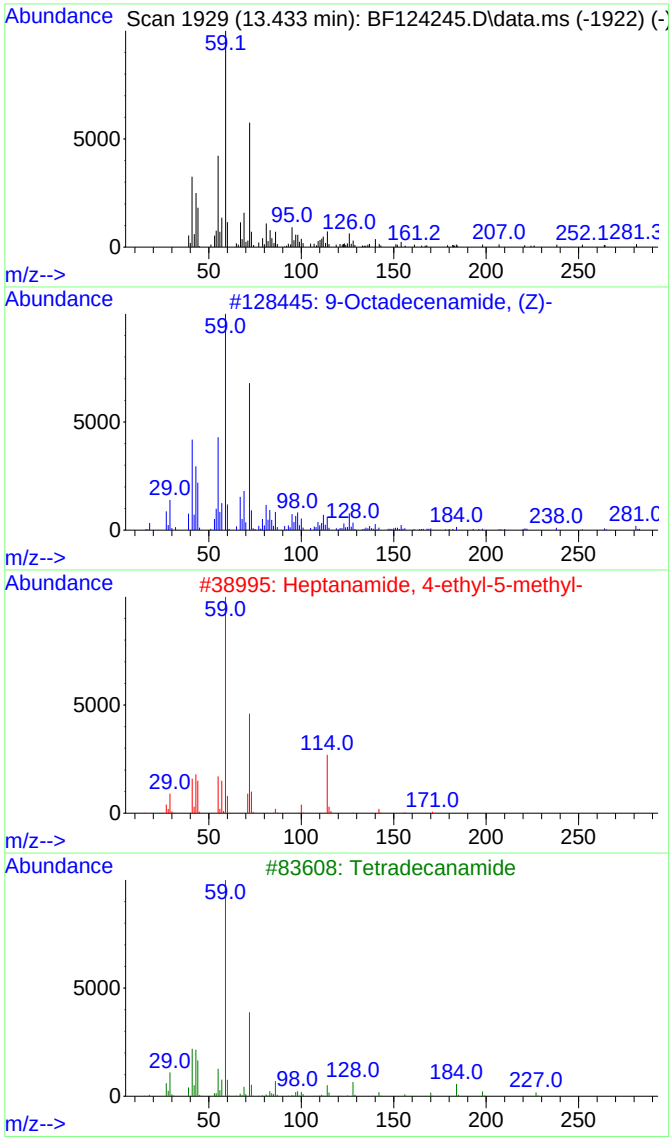
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

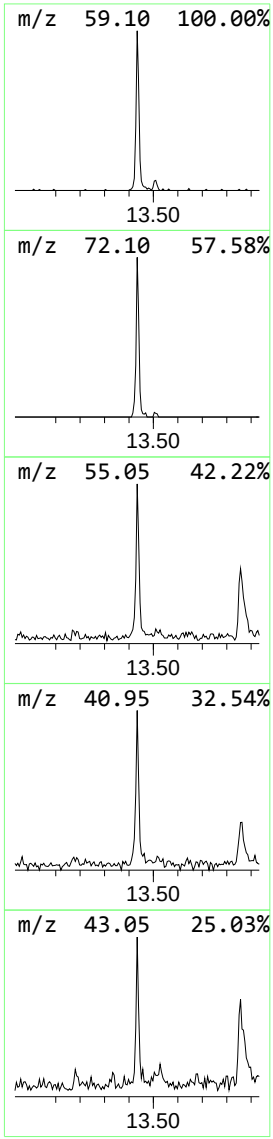
****

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.433	18.27 ng	275521	Chrysene-d12	14.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99
2	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	72
3	Tetradecanamide	227	C14H29NO	000638-58-4	56
4	Hexadecanamide	255	C16H33NO	000629-54-9	56
5	Undecanamide, 11-bromo-	263	C11H22BrNO	005875-26-3	53





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ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 17-B6(4-8)

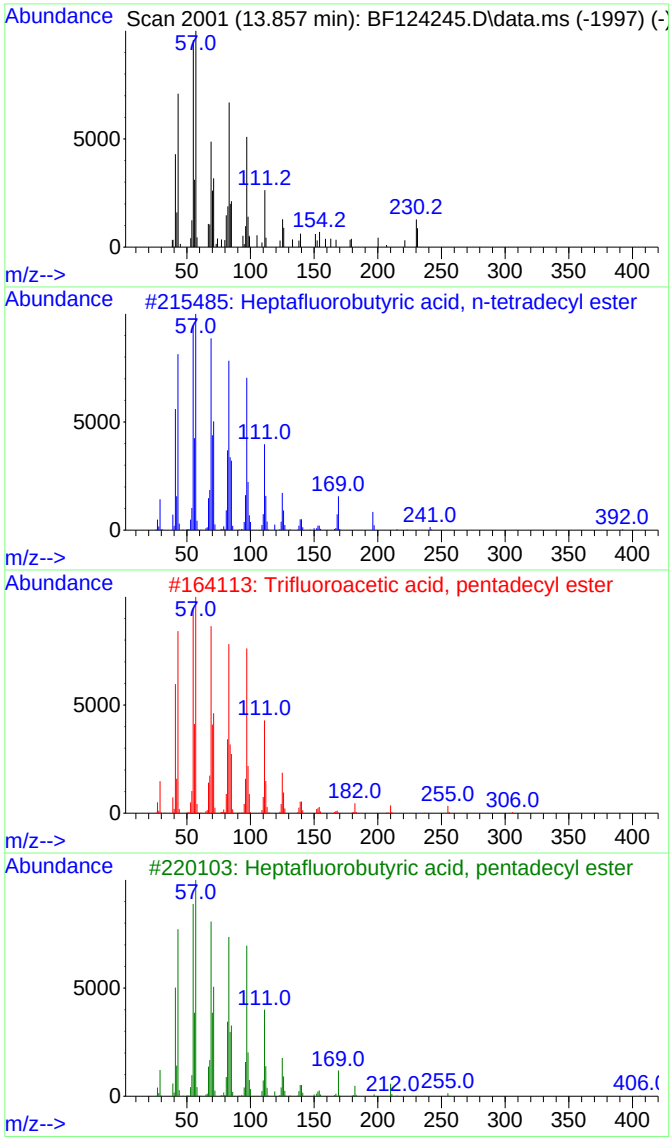
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

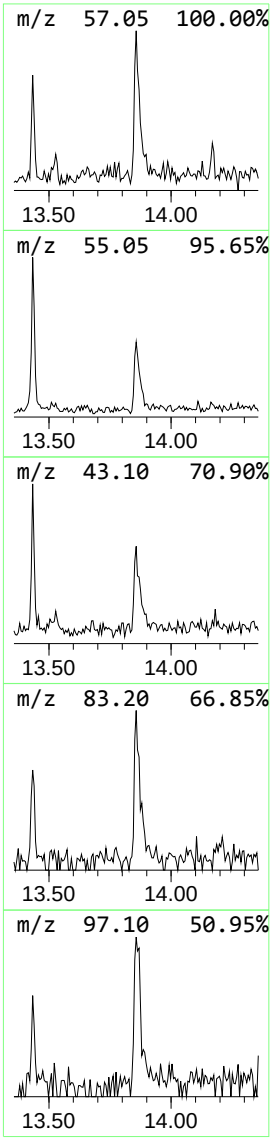
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Heptafluorobutyric acid, n-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	10.00 ng	150743	Chrysene-d12	14.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	90
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	90
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	90
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90





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Instrument : BNA_F
ClientSampleId : 17-B6(4-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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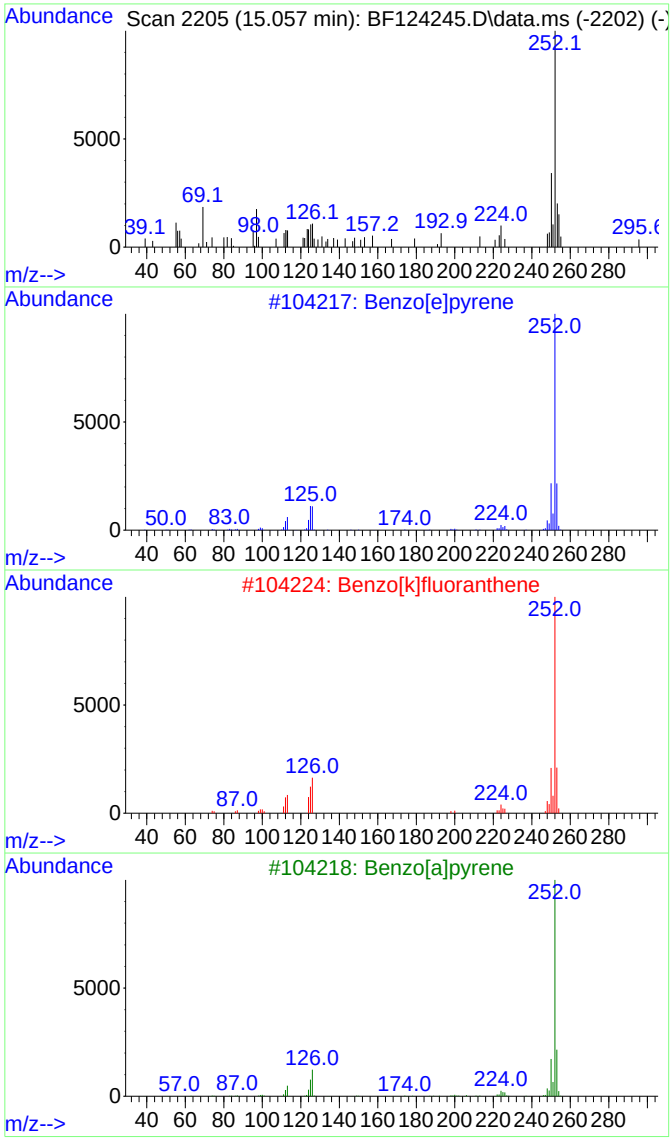
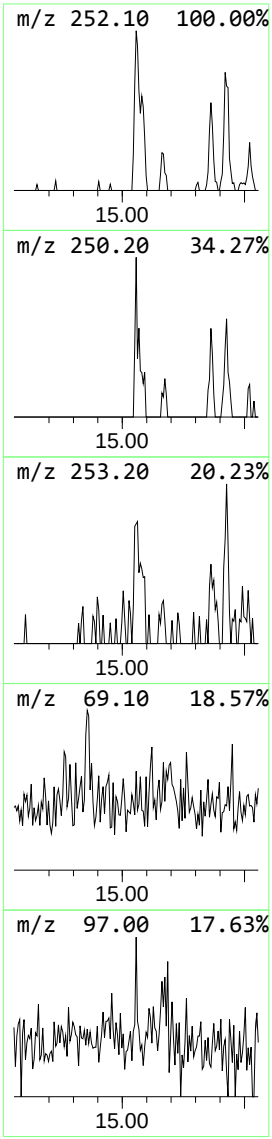
Peak Number 8 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.057	3.54 ng	50930	Perylene-d12	15.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	76
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	70
3	Benzo[a]pyrene	252	C20H12	000050-32-8	64
4	Perylene	252	C20H12	000198-55-0	59
5	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061021\
Data File : BF124245.D
Acq On : 10 Jun 2021 22:01
Operator : JU/CG
Sample : M2651-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 17-B6(4-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

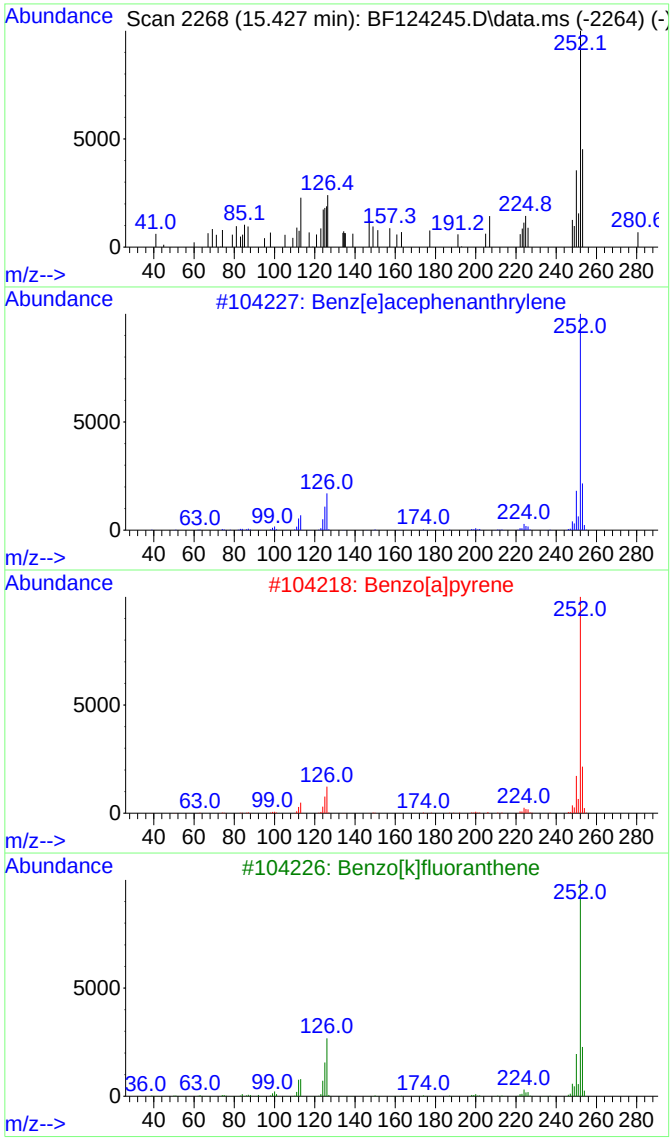
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

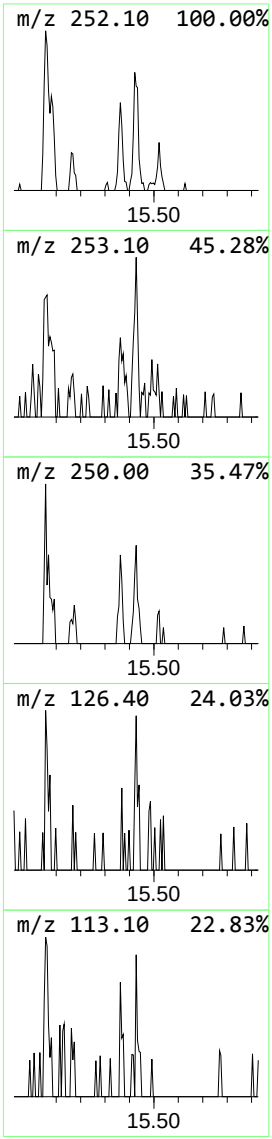
****

Peak Number 9 Perylene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.427	2.22 ng	31915	Perylene-d12	15.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	50
2	Benzo[a]pyrene	252	C20H12	000050-32-8	49
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	47
4	Perylene	252	C20H12	000198-55-0	43
5	Benzo[e]pyrene	252	C20H12	000192-97-2	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061021\
Data File : BF124245.D
Acq On : 10 Jun 2021 22:01
Operator : JU/CG
Sample : M2651-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
17-B6(4-8)

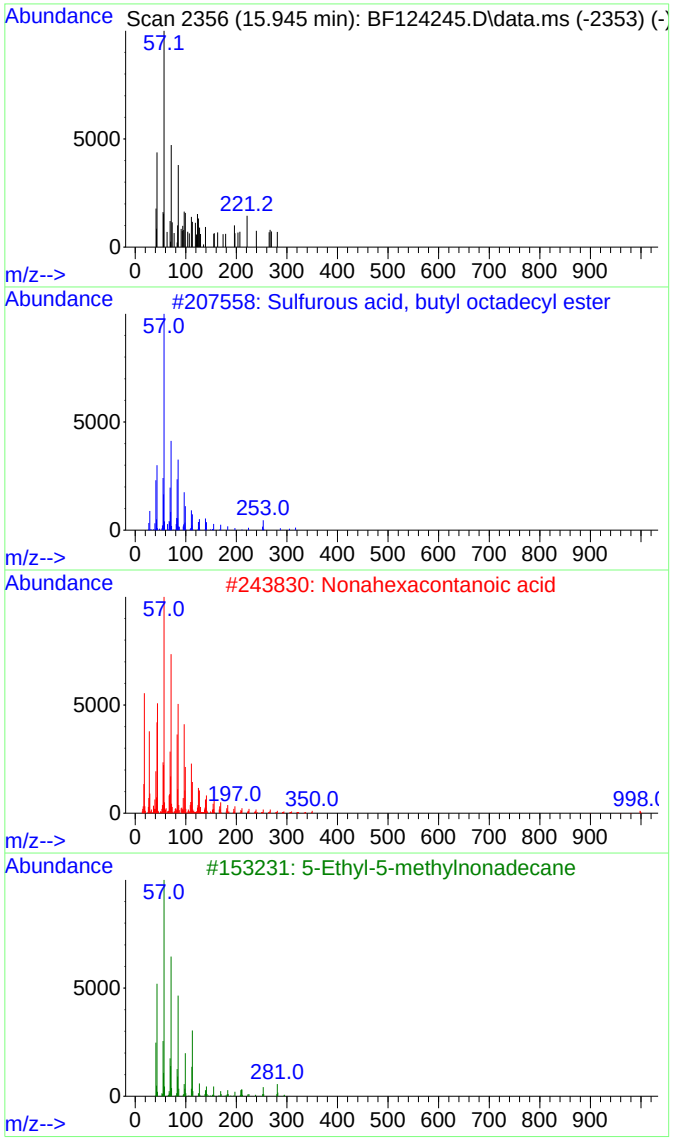
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

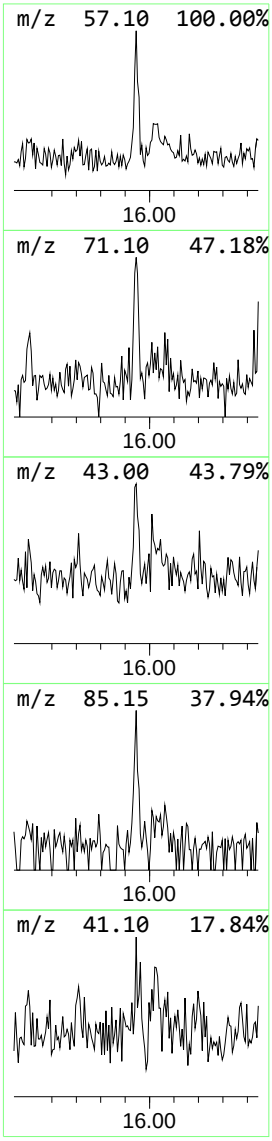
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Sulfurous acid, butyl octad... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.945	2.15 ng	30993	Perylene-d12	15.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	50
2	Nonahexacontanoic acid	999	C69H138O2	040710-32-5	50
3	5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	47
4	Tetracosane	338	C24H50	000646-31-1	43
5	Nonacosane	408	C29H60	000630-03-5	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061021\
Data File : BF124245.D
Acq On : 10 Jun 2021 22:01
Operator : JU/CG
Sample : M2651-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 17-B6(4-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.057	6.5	ng	74286	1	6.845	228660	20.0
Ethanol, 2-(2-e...	6.675	2.7	ng	30607	1	6.845	228660	20.0
n-Hexadecanoic ...	11.898	6.5	ng	112038	4	11.374	347472	20.0
unknown12.816	12.816	2.6	ng	39267	5	14.015	301632	20.0
9-Octadecenamid...	13.433	18.3	ng	275521	5	14.015	301632	20.0
Heptafluorobuty...	13.857	10.0	ng	150743	5	14.015	301632	20.0
Benzo[e]pyrene	15.057	3.5	ng	50930	6	15.492	287725	20.0
Perylene	15.427	2.2	ng	31915	6	15.492	287725	20.0
Sulfurous acid,...	15.945	2.1	ng	30993	6	15.492	287725	20.0