LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
Data File : BF099599.D
Acq On : 17 Oct 2017 23:36
Operator : SJ/JU
Sample : I5869-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-7D-10-11-17

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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.051	500	504	520	rVB	103042	128733	3.86%	0.530%
2	5.457	570	573	594	rVB	1498278	1375113	41.24%	5.665%
3	6.469	742	745	763	rBV	957460	853657	25.60%	3.517%
4	6.604	763	768	771	rBV	2618458	2425463	72.74%	9.992%
5	6.828	802	806	811	rBV	791806	662186	19.86%	2.728%
6	6.987	828	833	836	rBV	2424848	2387700	71.61%	9.836%
7	7.398	897	903	906	rBV	1792710	1847425	55.40%	7.611%
8	8.110	1020	1024	1027	rBV	1015913	884415	26.52%	3.643%
9	9.186	1201	1207	1210	rBV	3178002	3334528	100.00%	13.737%
10	9.575	1267	1273	1275	rBV	42992	35868	1.08%	0.148%
11	9.604	1275	1278	1281	rVV	135571	97628	2.93%	0.402%
12	9.657	1284	1287	1294	rVB	61458	46945	1.41%	0.193%
13	9.810	1309	1313	1316	rBV2	1109035	1250017	37.49%	5.150%
14	9.863	1319	1322	1325	rVB	1006487	912950	27.38%	3.761%
15	10.233	1379	1385	1388	rBV	402761	312108	9.36%	1.286%
16	10.275	1390	1392	1395	rVB2	39277	36260	1.09%	0.149%
17	10.486	1425	1428	1432	rBV3	56630	74884	2.25%	0.308%
18	10.657	1453	1457	1460	rBV	1365691	1260589	37.80%	5.193%
19	10.751	1470	1473	1475	rBV	64868	52961	1.59%	0.218%
20	10.775	1475	1477	1480	rVB	41282	42116	1.26%	0.174%
21	10.945	1502	1506	1510	rBV2	74019	106863	3.20%	0.440%
22	11.198	1547	1549	1551	rBV2	60429	59057	1.77%	0.243%
23	11.351	1571	1575	1577	rBV	767193	722600	21.67%	2.977%
24	11.375	1577	1579	1584	rVB	71593	88601	2.66%	0.365%
25	11.633	1619	1623	1627	rBV3	24317	47293	1.42%	0.195%
26	11.786	1644	1649	1654	rBV2	62633	111166	3.33%	0.458%
27	11.922	1667	1672	1676	rBV5	27607	43824	1.31%	0.181%
28	12.033	1688	1691	1695	rBV	37258	47589	1.43%	0.196%
29	12.180	1713	1716	1719	rBV2	41515	48971	1.47%	0.202%
30	12.927	1839	1843	1847	rBV	1886561	1887895	56.62%	7.777%
31	13.992	2020	2024	2027	rBV	584772	556821	16.70%	2.294%
32	14.421	2094	2097	2102	rBV4	21876	37958	1.14%	0.156%
33	14.592	2123	2126	2130	rBV	65367	63793	1.91%	0.263%
34	14.727	2145	2149	2154	rBV5	26068	39147	1.17%	0.161%

LSC Area Percent Report

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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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.451	2266	2272	2280	rVB	503452	629885	18.89%	2.595%
36	15.857	2338	2341	2345	rBV2	31125	42248	1.27%	0.174%
37	16.115	2377	2385	2392	rBV3	15398	34821	1.04%	0.143%
38	16.351	2420	2425	2430	rBV2	34996	58586	1.76%	0.241%
39	16.615	2464	2470	2479	rVB	39531	75388	2.26%	0.311%
40	16.927	2518	2523	2529	rVB4	28008	56051	1.68%	0.231%
41	17.151	2553	2561	2571	rBV	186884	397786	11.93%	1.639%
42	17.609	2633	2639	2649	rVB4	25317	68507	2.05%	0.282%
43	17.821	2664	2675	2690	rBV2	383513	989418	29.67%	4.076%
44	18.421	2773	2777	2786	rVB6	16257	38308	1.15%	0.158%

Sum of corrected areas: 24274122

LSC Report - Integrated Chromatogram

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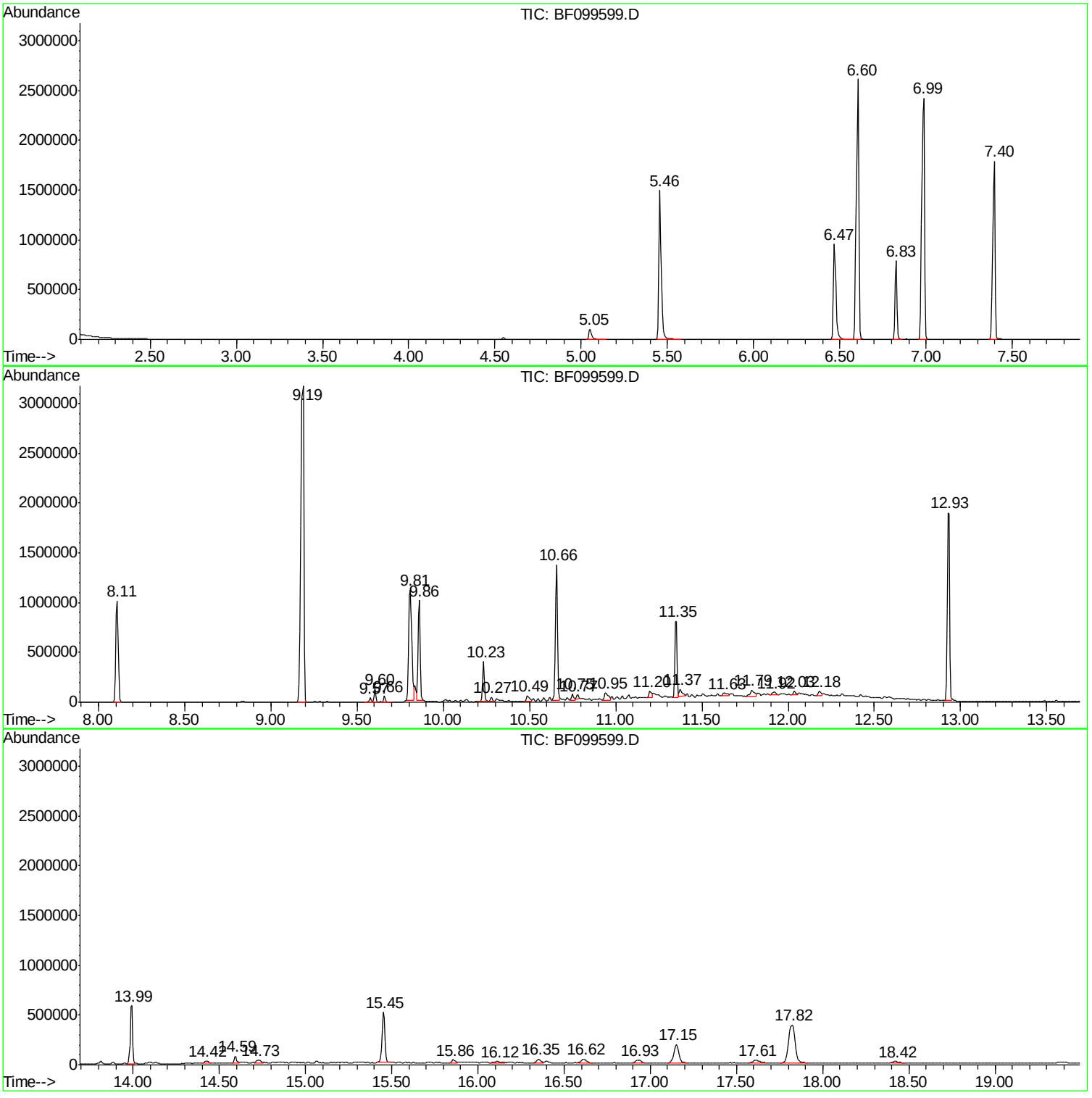
Operator : SJ/JU
Sample : I5869-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-7D-10-11-17

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Data File : BF099599.D
Acq On : 17 Oct 2017 23:36
Operator : SJ/JU
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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-7D-10-11-17

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

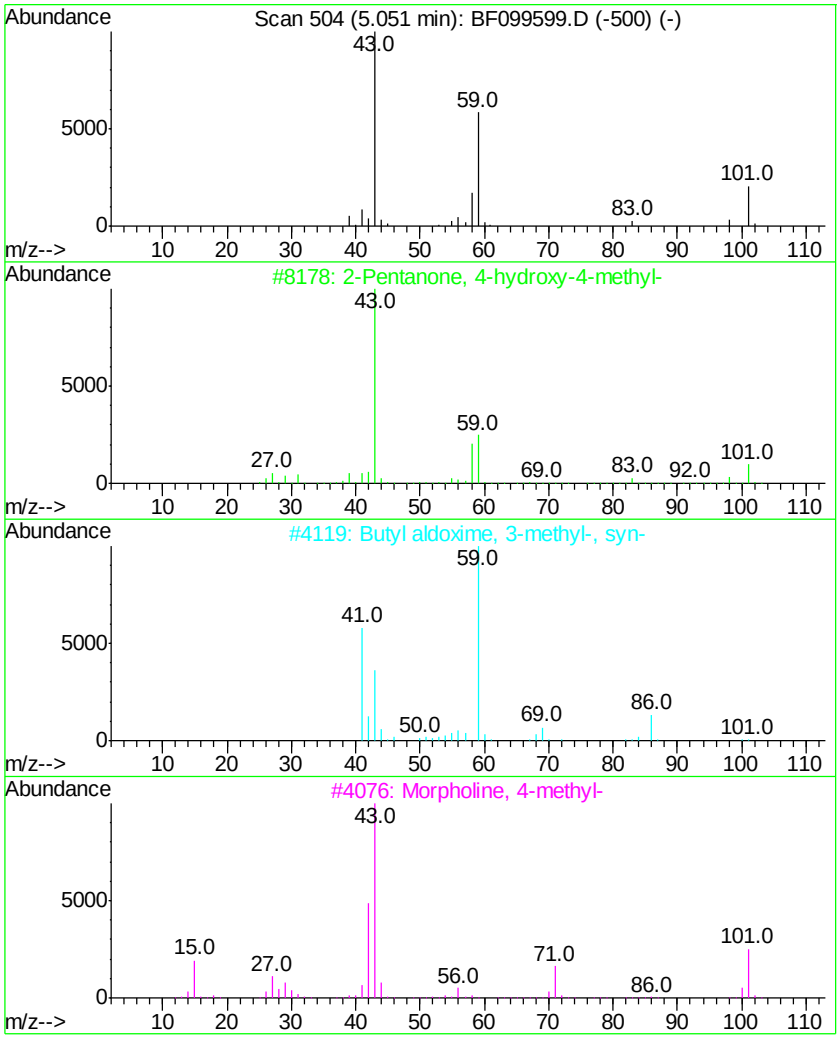
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

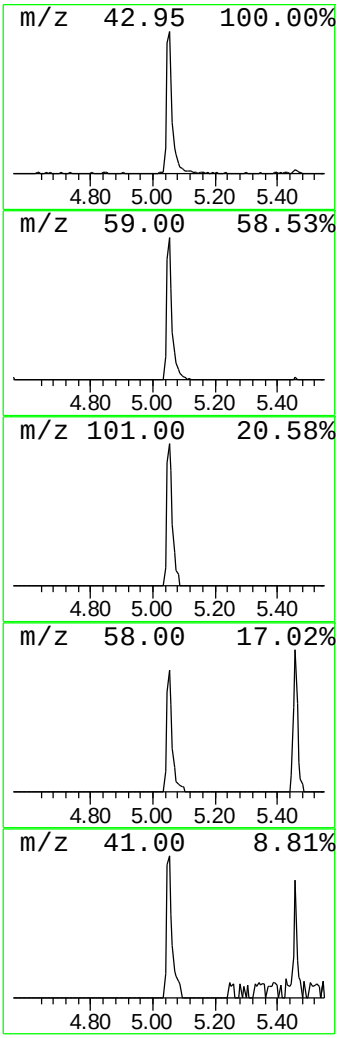
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	3.89 ng	128733	1,4-Dichlorobenzene-d4	6.83

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	25
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Library Search Compound Report

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Operator : SJ/JU
Sample : I5869-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-7D-10-11-17

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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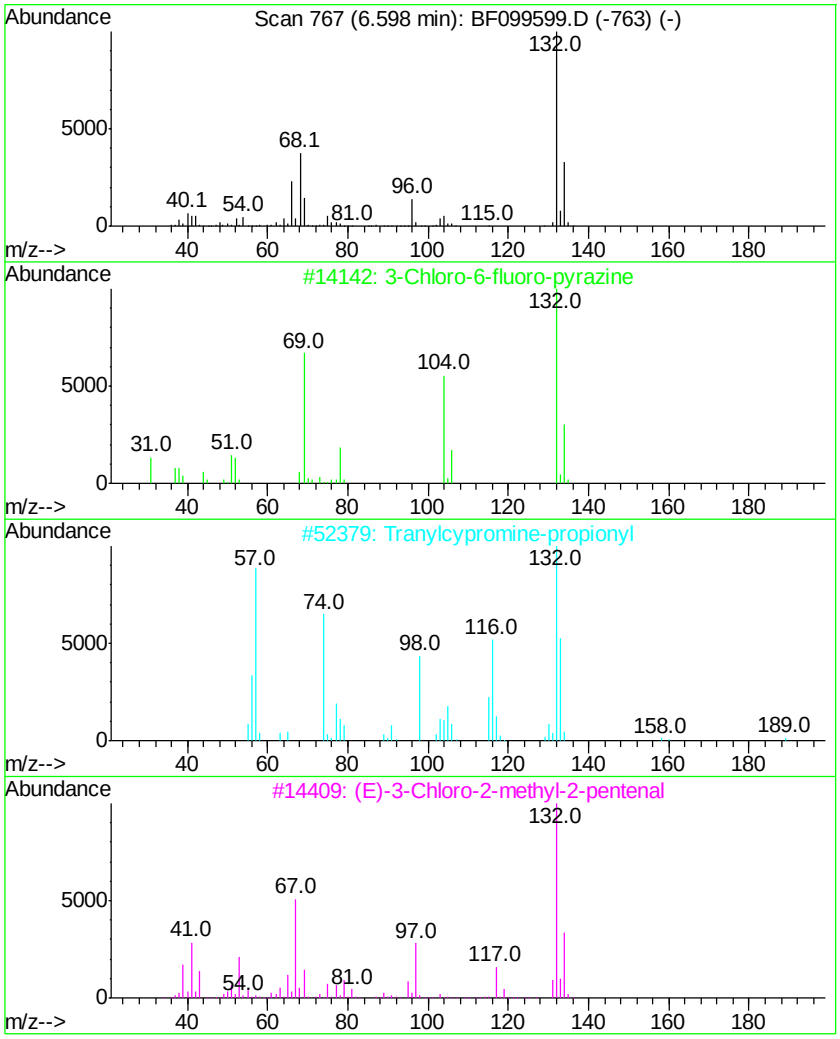
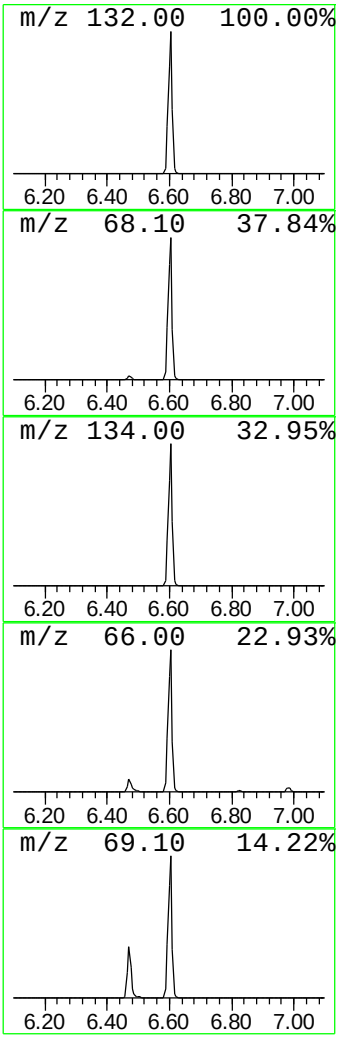
****

Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	73.26 ng	2425460	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Sample : I5869-07
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Instrument : BNA_F
ClientSampleId : MW-7D-10-11-17

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

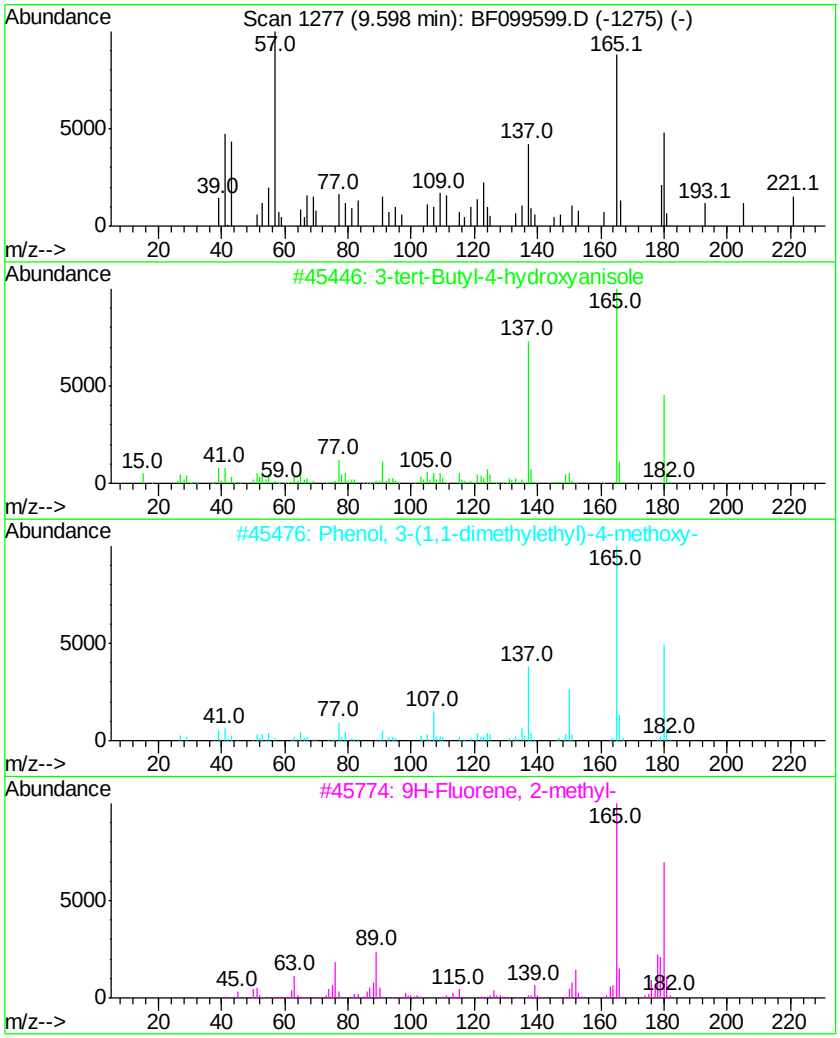
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

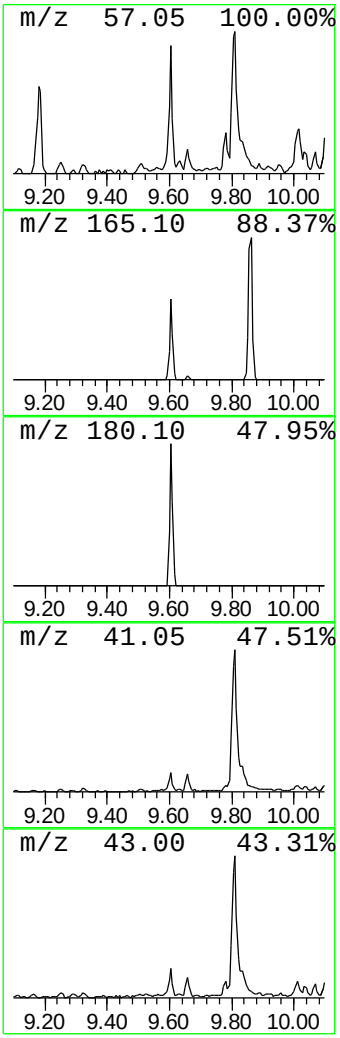
****

Peak Number 4 3-tert-Butyl-4-hydroxyanisole Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.60	2.14 ng	97628	Acenaphthene-d10	9.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	83
2	Phenol, 3-(1,1-dimethylethyl)-4-...	180	C11H16O2	000088-32-4	76
3	9H-Fluorene, 2-methyl-	180	C14H12	001430-97-3	58
4	5-tert-Butyl-2-methylbenzenethiol	180	C11H16S	007340-90-1	52
5	2-Amino-4-(tert-butyl)thiophene-...	180	C9H12N2S	010413-34-0	52





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Misc :
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Instrument : BNA_F
ClientSampleId : MW-7D-10-11-17

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

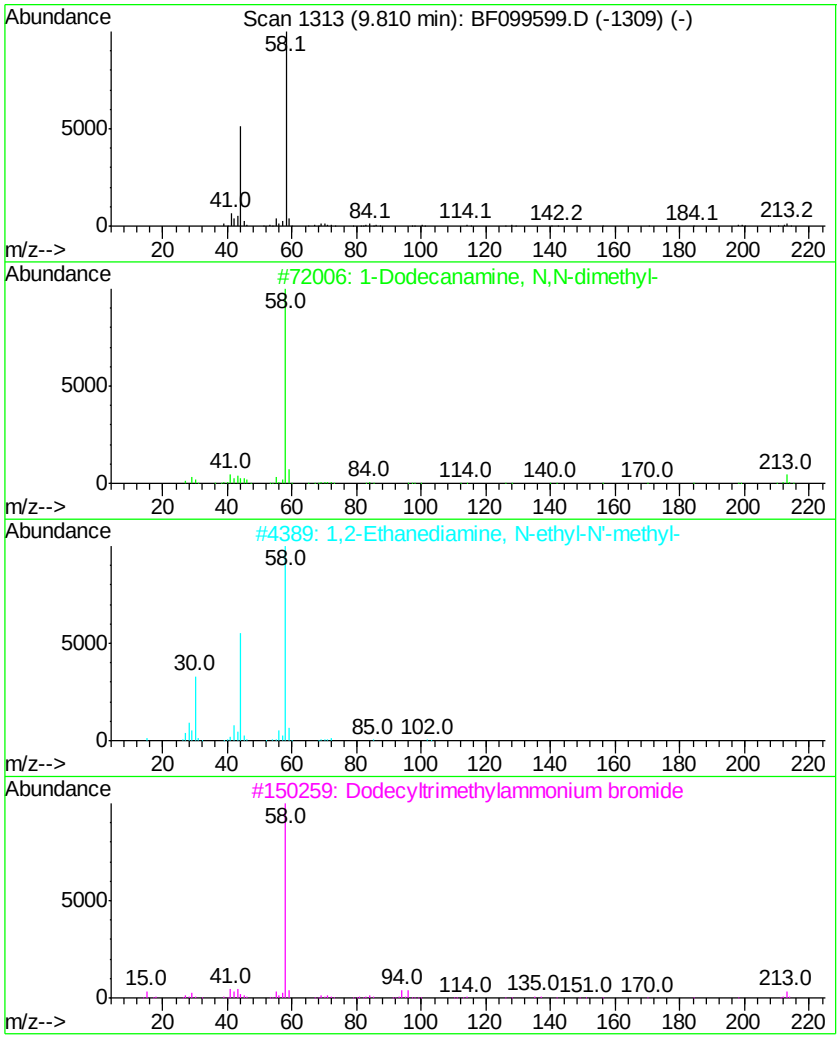
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

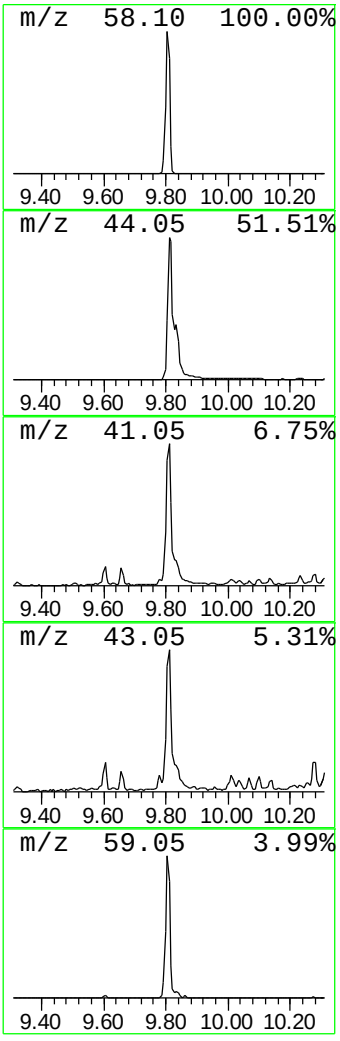
****

Peak Number 5 1-Dodecanamine, N,N-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.81	27.38 ng	1250020	Acenaphthene-d10	9.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanamine, N,N-dimethyl-	213	C14H31N	000112-18-5	50
2	1,2-Ethanediamine, N-ethyl-N'-me...	102	C5H14N2	000111-37-5	50
3	Dodecyltrimethylammonium bromide	307	C15H34BrN	001119-94-4	50
4	Cetrimonium Bromide	363	C19H42BrN	000057-09-0	50
5	1-Nonanamine, N,N-dimethyl-	171	C11H25N	017373-27-2	40





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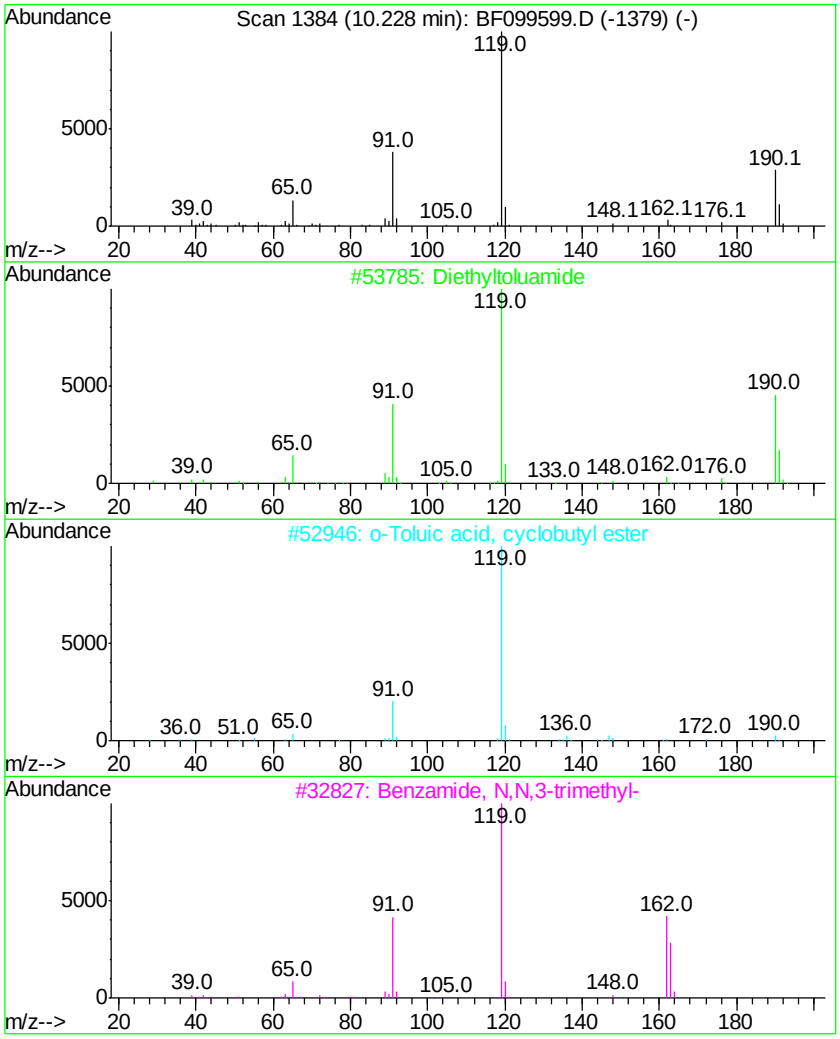
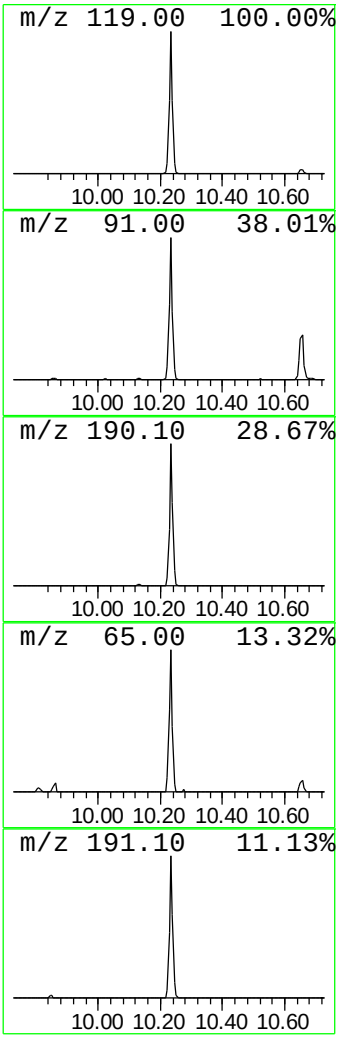
Peak Number 6 Diethyltoluamide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.23	6.84 ng	312108	Acenaphthene-d10	9.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyltoluamide	191	C12H17NO	000134-62-3	95
2	o-Toluic acid, cyclobutyl ester	190	C12H14O2	1000292-22-3	72
3	Benzamide, N,N,3-trimethyl-	163	C10H13NO	006935-65-5	59
4	m-Toluic acid, 4-cyanophenyl ester	237	C15H11NO2	1000307-56-9	58
5	4-Methylbenzoic acid, pentafluor...	302	C14H7F5O2	1000354-15-1	58





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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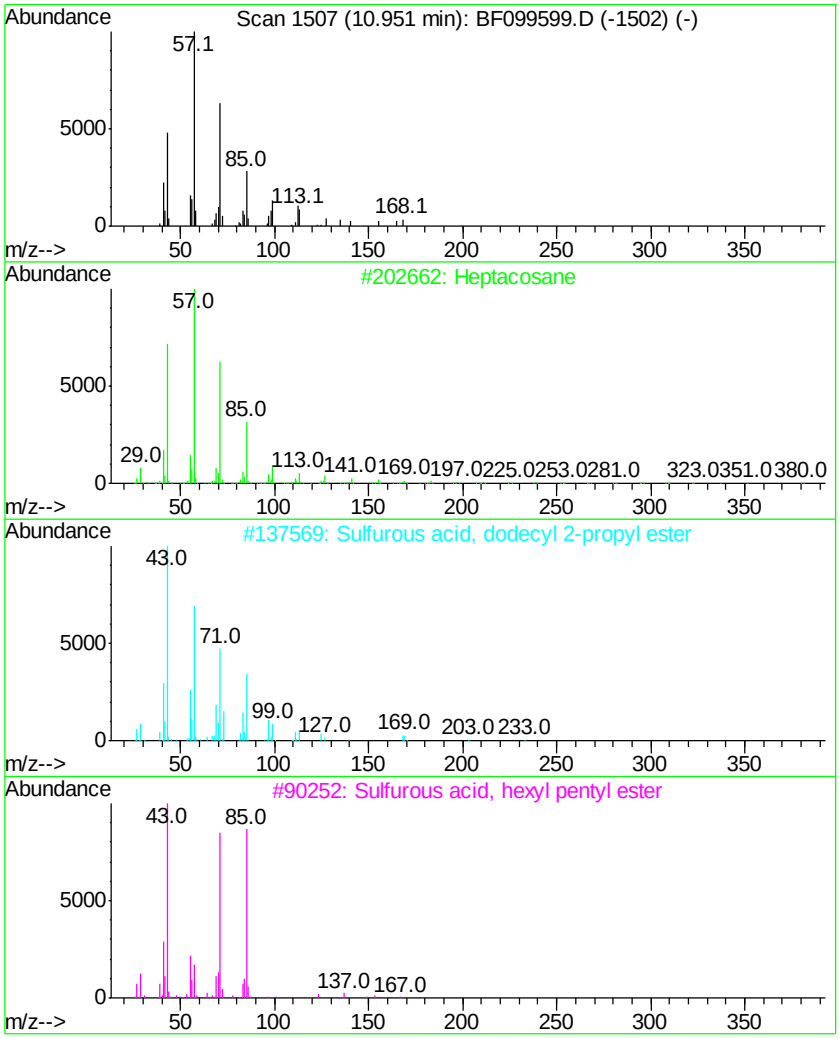
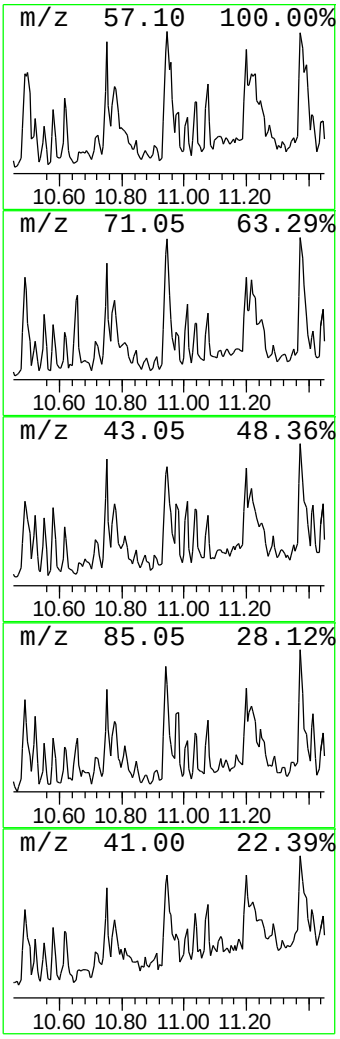
Peak Number 7 Heptacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.95	2.96 ng	106863	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	90
2	Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	72
3	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	58
4	10-Methylnonadecane	282	C20H42	056862-62-5	58
5	Heptadecane	240	C17H36	000629-78-7	52





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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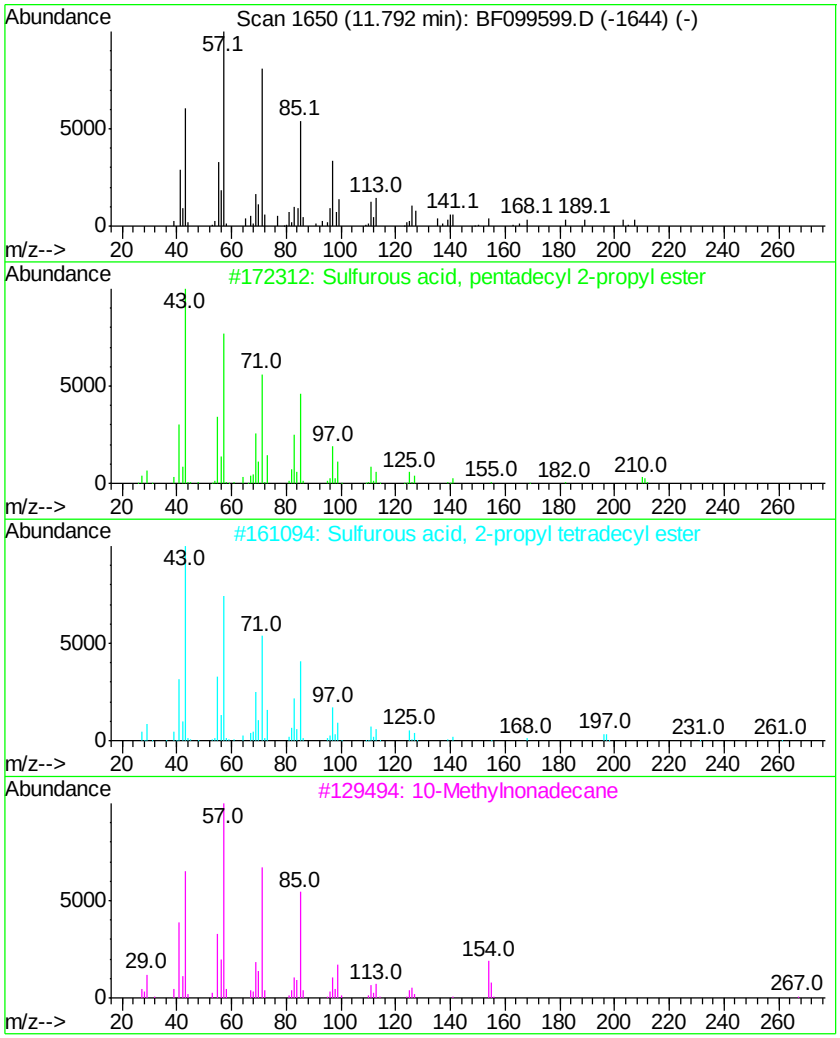
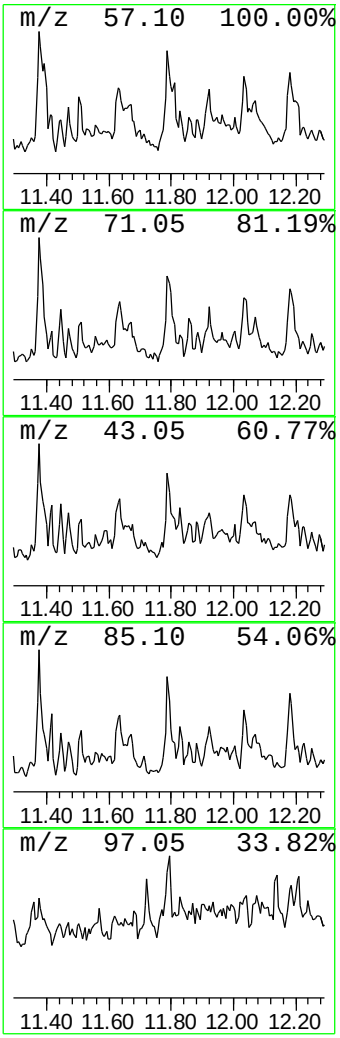
Peak Number 8 Sulfurous acid, pentadecyl ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	3.08 ng	111166	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	80
2	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	80
3	10-Methylnonadecane	282	C20H42	056862-62-5	72
4	9-methylheptadecane	254	C18H38	026741-18-4	68
5	Tetracosane	338	C24H50	000646-31-1	64





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Sample : I5869-07
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Instrument : BNA_F
ClientSampleId : MW-7D-10-11-17

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

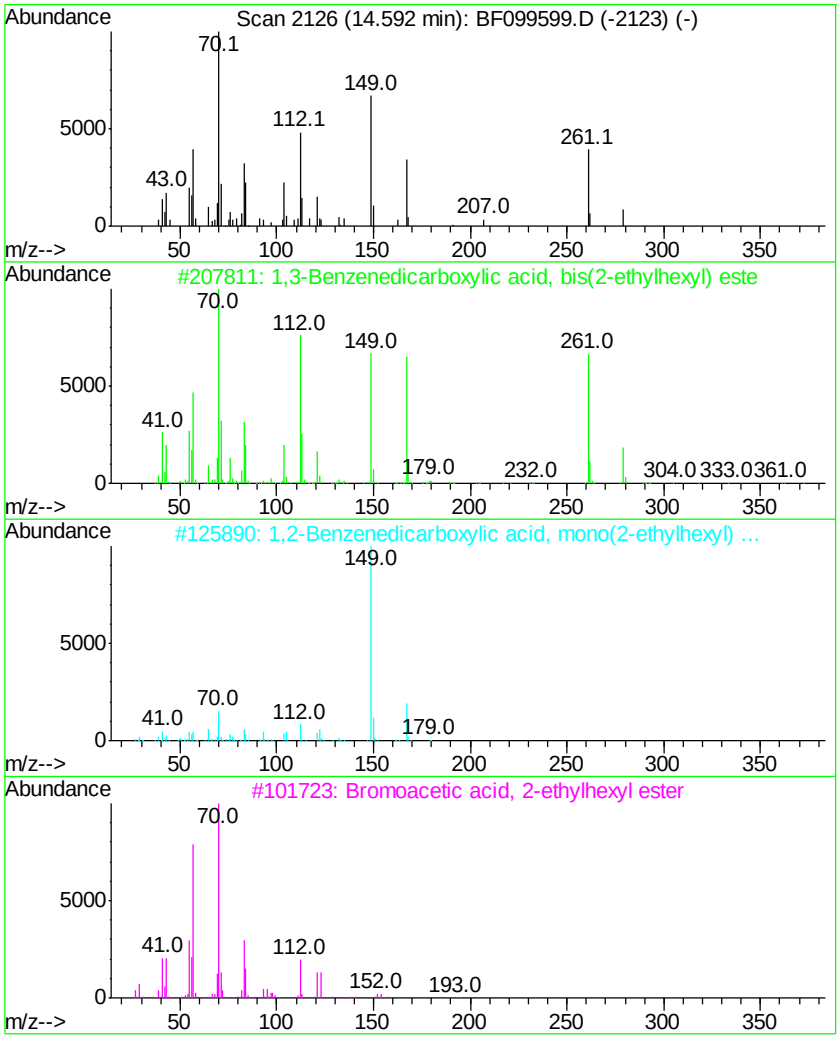
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

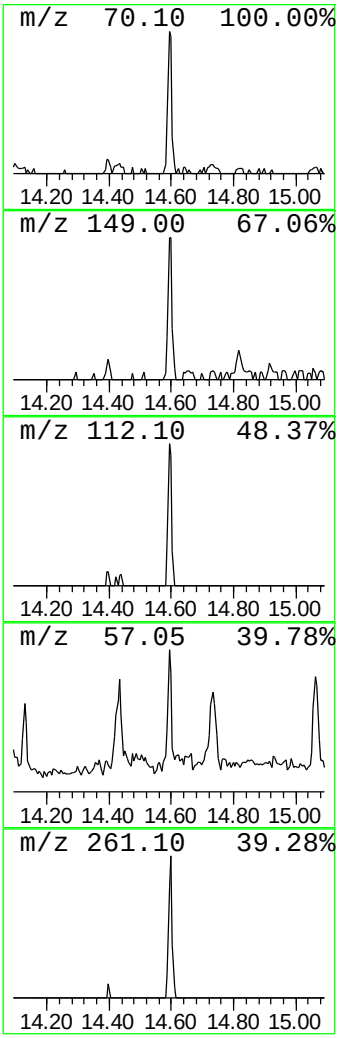
****

Peak Number 9 1,3-Benzenedicarboxylic aci... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	2.29 ng	63793	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	52
2	1,2-Benzenedicarboxylic acid, mo...	278	C16H22O4	004376-20-9	32
3	Bromoacetic acid, 2-ethylhexyl e...	250	C10H19BrO2	068144-73-0	27
4	Diisooctyl phthalate	390	C24H38O4	000131-20-4	22
5	Phthalic acid, 1-naphthyl octyl ...	404	C26H28O4	1000315-23-5	22





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Data File : BF099599.D
Acq On : 17 Oct 2017 23:36
Operator : SJ/JU
Sample : I5869-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-7D-10-11-17

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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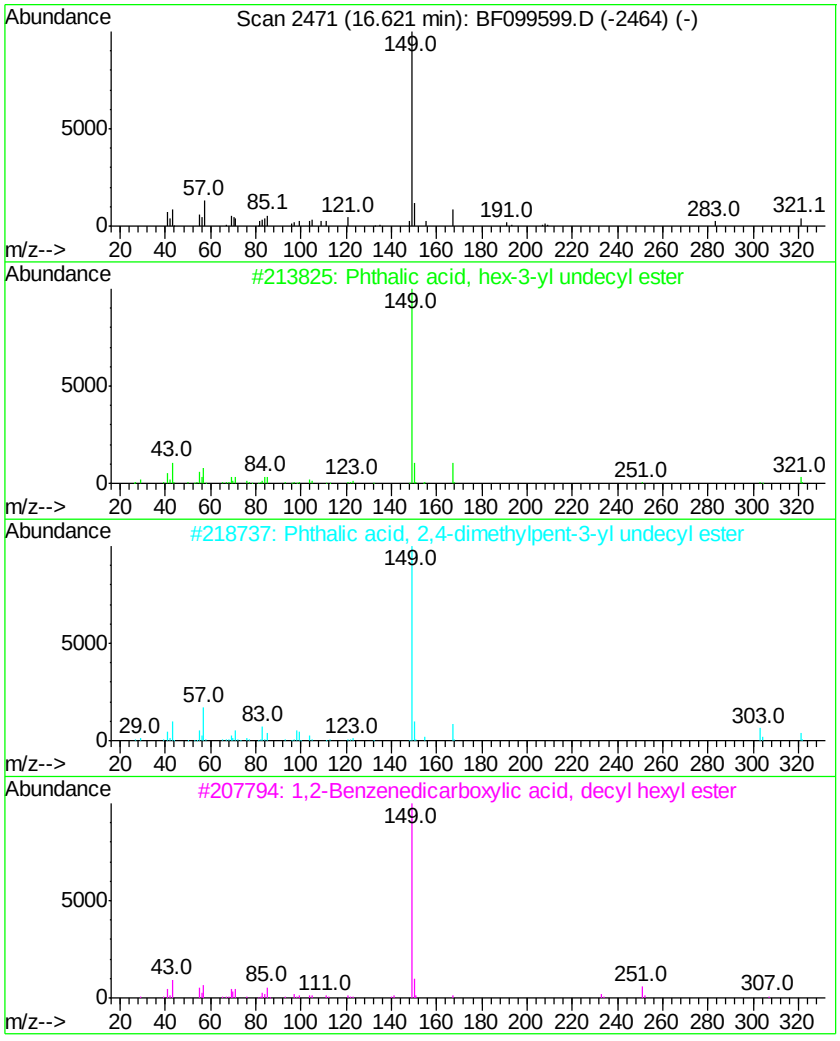
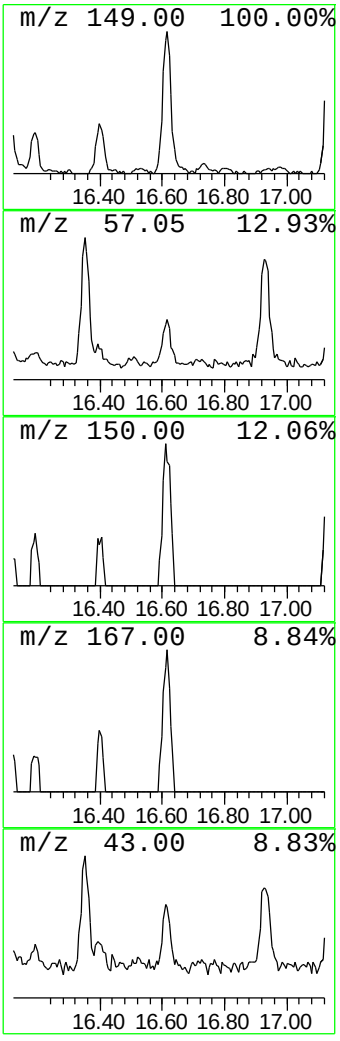
Peak Number 10 Phthalic acid, hex-3-yl und... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.62	2.39 ng	75388	Perylene-d12	15.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, hex-3-yl undecyl ...	404	C25H40O4	1000356-96-2	86
2	Phthalic acid, 2,4-dimethylpent-...	418	C26H42O4	1000356-85-0	83
3	1,2-Benzenedicarboxylic acid, de...	390	C24H38O4	025724-58-7	80
4	Phthalic acid, decyl hex-3-yl ester	390	C24H38O4	1000356-96-1	78
5	Phthalic acid, dodecyl 2-propylp...	452	C29H40O4	1000357-02-7	72





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Data File : BF099599.D
Acq On : 17 Oct 2017 23:36
Operator : SJ/JU
Sample : I5869-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-7D-10-11-17

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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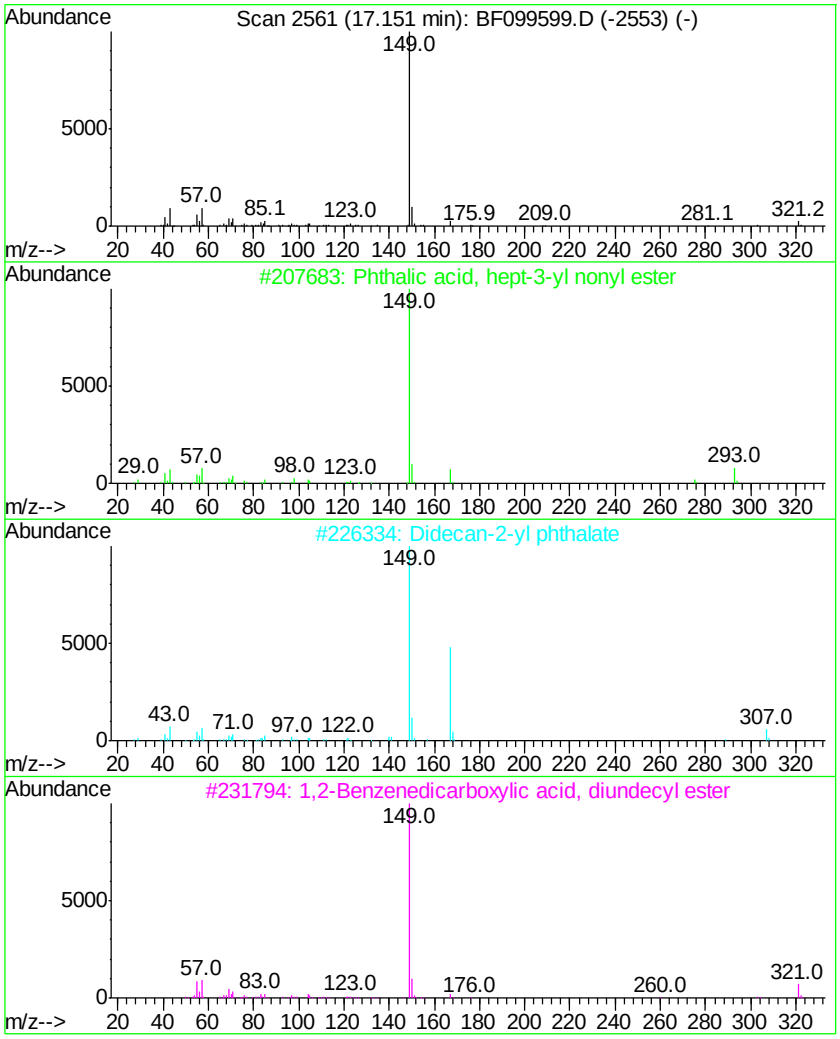
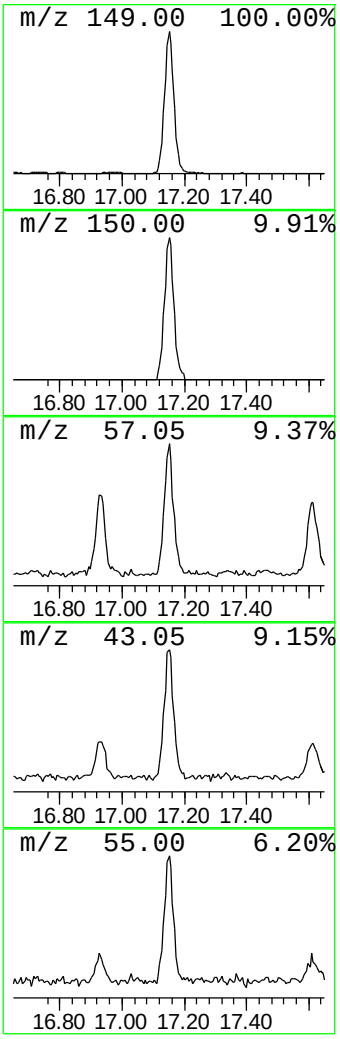
Peak Number 11 Phthalic acid, hept-3-yl no... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.15	12.63 ng	397786	Perylene-d12	15.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, hept-3-yl nonyl e...	390	C24H38O4	1000356-99-3	86
2	Didecan-2-yl phthalate	446	C28H46O4	028029-89-2	86
3	1,2-Benzenedicarboxylic acid, di...	474	C30H50O4	003648-20-2	83
4	Phthalic acid, dodecyl nonyl ester	460	C29H48O4	1000308-92-6	80
5	Phthalic acid, hept-3-yl octyl e...	376	C23H36O4	1000356-99-2	78





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Data File : BF099599.D
Acq On : 17 Oct 2017 23:36
Operator : SJ/JU
Sample : I5869-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-7D-10-11-17

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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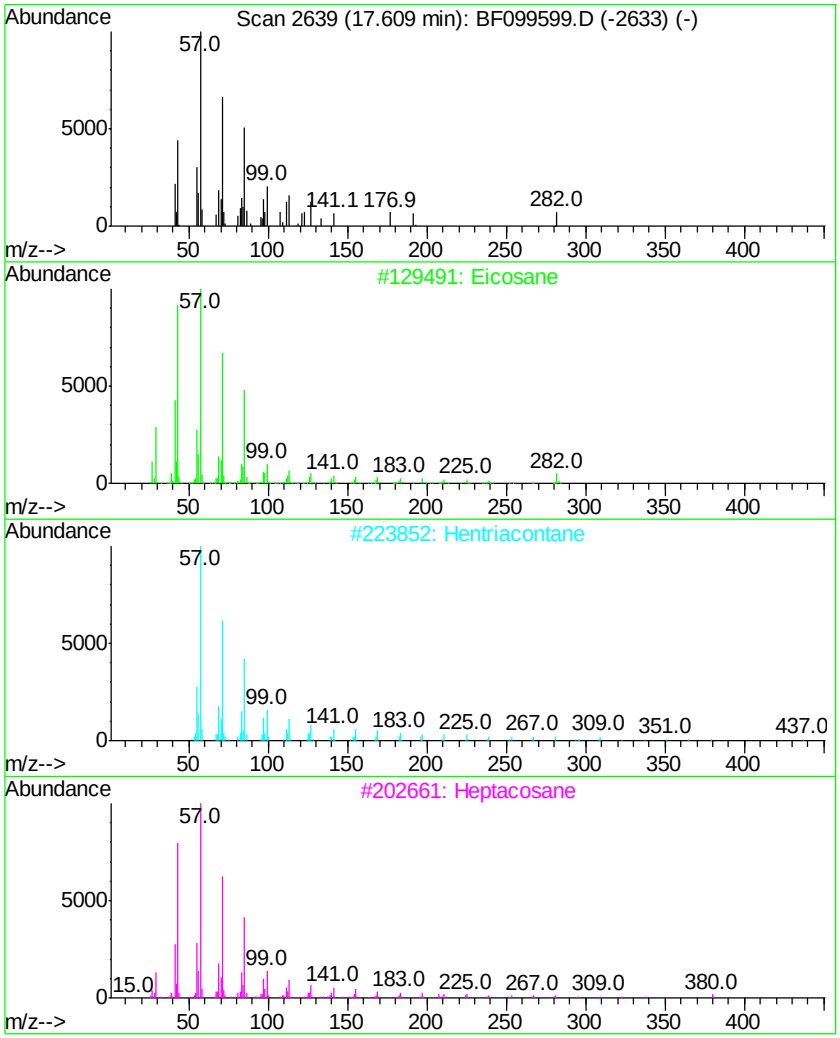
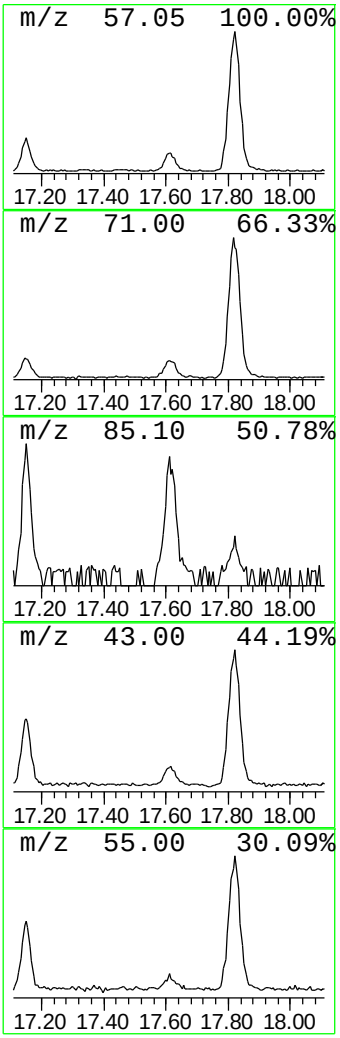
Peak Number 12 Eicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.61	2.18 ng	68507	Perylene-d12	15.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Hentriacontane	437	C31H64	000630-04-6	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Octacosane	394	C28H58	000630-02-4	91





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Data File : BF099599.D
Acq On : 17 Oct 2017 23:36
Operator : SJ/JU
Sample : I5869-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-7D-10-11-17

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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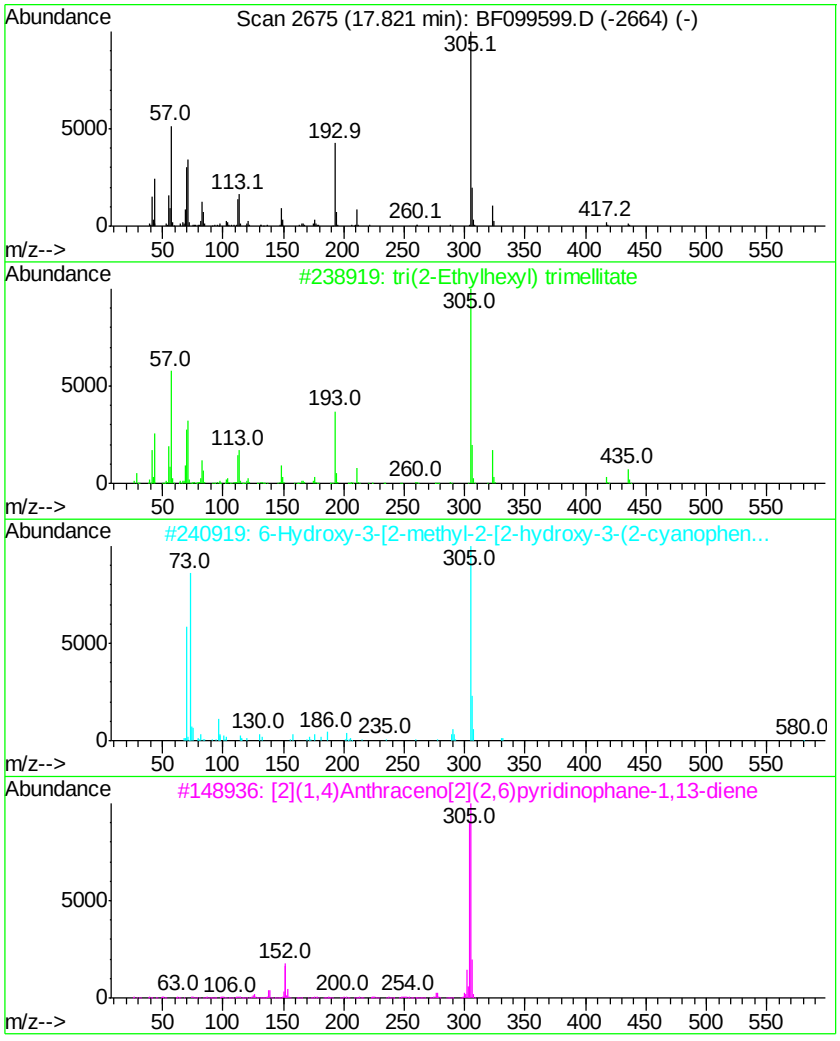
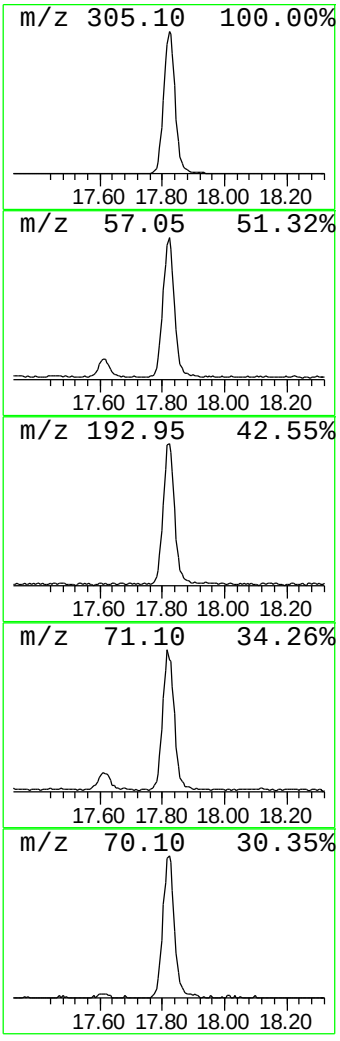
Peak Number 13 unknown17.82 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.82	31.42 ng	989418	Perylene-d12	15.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	tri(2-Ethylhexyl) trimellitate	546	C33H54O6	003319-31-1	49
2	6-Hydroxy-3-[2-methyl-2-[2-hydro...	595	C31H49N3O3Si3	1000292-78-8	20
3	[2](1,4)Anthraceno[2](2,6)pyridi...	305	C23H15N	106727-24-6	9
4	[1,2,4]Triazolo[1,5-a]pyrimidine...	306	C17H18N6	1000350-66-1	9
5	2H-Furo[2,3-H]chromen-2-one, 8,9...	305	C19H15NO3	1000271-14-0	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101717\
Data File : BF099599.D
Acq On : 17 Oct 2017 23:36
Operator : SJ/JU
Sample : I5869-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-7D-10-11-17

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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-hy...	5.05	3.9	ng	128733	1	6.83	662186	20.0
unknown6.60	6.60	73.3	ng	2425460	1	6.83	662186	20.0
3-tert-Butyl-4-hy...	9.60	2.1	ng	97628	3	9.86	912950	20.0
1-Dodecanamine, N...	9.81	27.4	ng	1250020	3	9.86	912950	20.0
Diethyltoluamide	10.23	6.8	ng	312108	3	9.86	912950	20.0
Heptacosane	10.95	3.0	ng	106863	4	11.35	722600	20.0
Sulfurous acid, p...	11.79	3.1	ng	111166	4	11.35	722600	20.0
1,3-Benzenedicarb...	14.59	2.3	ng	63793	5	13.99	556821	20.0
Phthalic acid, he...	16.62	2.4	ng	75388	6	15.45	629885	20.0
Phthalic acid, he...	17.15	12.6	ng	397786	6	15.45	629885	20.0
Eicosane	17.61	2.2	ng	68507	6	15.45	629885	20.0
unknown17.82	17.82	31.4	ng	989418	6	15.45	629885	20.0