LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032017\
Data File : BF093778.D
Acq On : 20 Mar 2017 21:42
Operator : SJ/MA
Sample : I2304-07 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SPA-B4(0-5)

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-BF032017.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	2.104	16	19	23	rVB	54191	84154	2.19%	0.223%
2	3.121	105	108	114	rVB	34549	63884	1.66%	0.169%
3	5.007	270	273	283	rVB	547965	689421	17.92%	1.824%
4	5.430	307	310	313	rBV	3103933	3074565	79.94%	8.135%
5	5.842	343	346	348	rVB	42508	42806	1.11%	0.113%
6	6.459	397	400	403	rBV	2596335	3523904	91.62%	9.323%
7	6.596	410	412	415	rBV	2734411	3535994	91.93%	9.355%
8	6.836	430	433	435	rBV	1686162	1420221	36.92%	3.758%
9	6.996	444	447	449	rBV	2737040	2811225	73.09%	7.438%
10	7.396	479	482	484	rBV	2522134	2406259	62.56%	6.366%
11	7.636	499	503	506	rVB3	54701	108888	2.83%	0.288%
12	7.865	518	523	524	rBV3	40675	74561	1.94%	0.197%
13	8.116	543	545	548	rBV	1684037	1831883	47.63%	4.847%
14	8.230	553	555	558	rVB	34228	42619	1.11%	0.113%
15	8.562	582	584	586	rBV	47516	54276	1.41%	0.144%
16	8.722	596	598	602	rBV	44806	85115	2.21%	0.225%
17	8.825	605	607	609	rVB	29404	39116	1.02%	0.103%
18	8.928	614	616	621	rVB4	22176	40795	1.06%	0.108%
19	9.156	635	636	637	rBV	57896	45075	1.17%	0.119%
20	9.202	637	640	642	rVB	3463588	3846308	100.00%	10.176%
21	9.293	645	648	650	rBV	117060	125188	3.25%	0.331%
22	9.453	660	662	666	rVB2	39670	60060	1.56%	0.159%
23	9.533	666	669	672	rBV3	56449	143907	3.74%	0.381%
24	9.590	672	674	675	rVV	395937	357029	9.28%	0.945%
25	9.613	675	676	678	rVV	112463	113792	2.96%	0.301%
26	9.648	678	679	684	rVB4	27930	49835	1.30%	0.132%
27	9.819	693	694	696	rVB	157735	117289	3.05%	0.310%
28	9.876	696	699	701	rBV	1550672	1941054	50.47%	5.136%
29	10.082	712	717	718	rBV4	49056	103557	2.69%	0.274%
30	10.139	721	722	724	rVB2	54145	62138	1.62%	0.164%
31	10.288	730	735	736	rBV5	53920	104762	2.72%	0.277%
32	10.322	736	738	739	rVB	104585	130093	3.38%	0.344%
33	10.436	745	748	750	rBV3	23552	43114	1.12%	0.114%
34	10.539	754	757	760	rBV	152890	180319	4.69%	0.477%

LSC Area Percent Report

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Sample : I2304-07 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SPA-B4(0-5)

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

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Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	10.619	763	764	765	rBV	39279	43161	1.12%	0.114%
36	10.653	765	767	769	rVB	1731850	1572624	40.89%	4.161%
37	10.802	777	780	783	rBV	280891	447066	11.62%	1.183%
38	10.985	794	796	798	rBV2	33194	47690	1.24%	0.126%
39	11.111	805	807	810	rBV3	27499	56048	1.46%	0.148%
40	11.236	816	818	819	rBV2	182723	159969	4.16%	0.423%
41	11.271	819	821	823	rVB	181555	201844	5.25%	0.534%
42	11.351	825	828	829	rBV	1633676	1612249	41.92%	4.266%
43	11.614	849	851	853	rBV	71489	85241	2.22%	0.226%
44	11.659	853	855	858	rVB	170046	159891	4.16%	0.423%
45	11.842	867	871	873	rBV4	57114	180539	4.69%	0.478%
46	11.956	880	881	887	rBV4	51549	126839	3.30%	0.336%
47	12.345	913	915	917	rBV	91820	121868	3.17%	0.322%
48	12.562	932	934	935	rBV2	80069	100271	2.61%	0.265%
49	12.928	964	966	969	rBV	2301758	2295104	59.67%	6.072%
50	13.831	1043	1045	1052	rBV	159879	375225	9.76%	0.993%
51	13.968	1055	1057	1059	rVV	965232	1052451	27.36%	2.785%
52	15.385	1178	1181	1183	rVB	706236	1020704	26.54%	2.701%
53	16.071	1238	1241	1249	rVB3	153233	428134	11.13%	1.133%
54	16.471	1273	1276	1281	rVB	183123	356127	9.26%	0.942%

Sum of corrected areas: 37796251

LSC Report - Integrated Chromatogram

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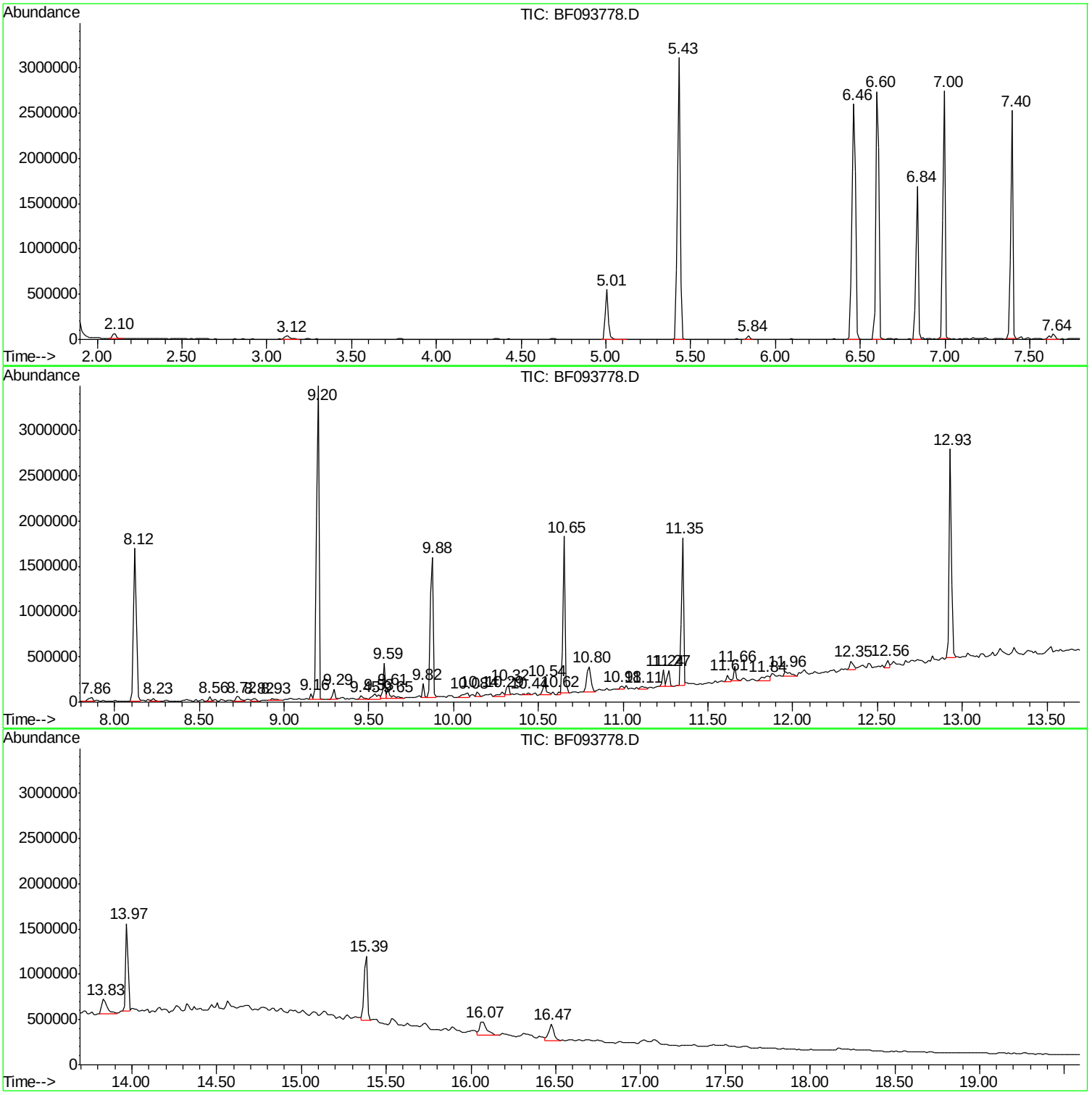
Data File : BF093778.D
Acq On : 20 Mar 2017 21:42
Operator : SJ/MA
Sample : I2304-07 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPA-B4(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032017\
Data File : BF093778.D
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Operator : SJ/MA
Sample : I2304-07 2X
Misc :
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Instrument : BNA_F
ClientSampleId : SPA-B4(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

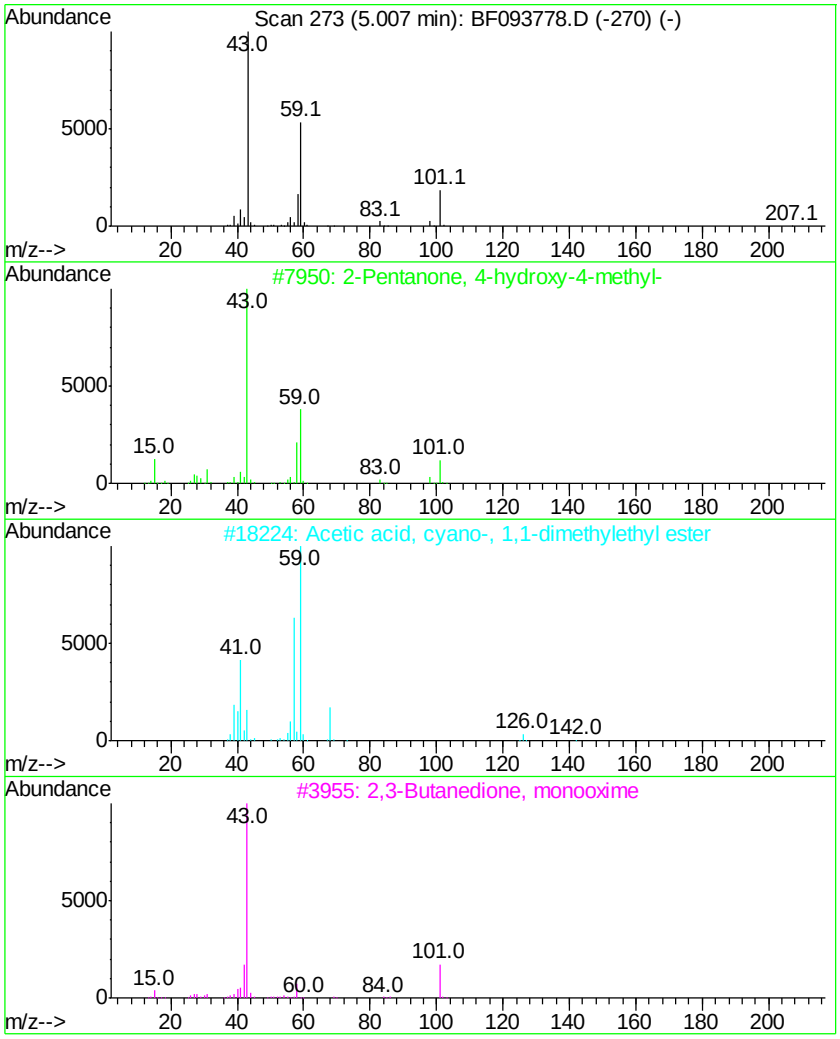
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

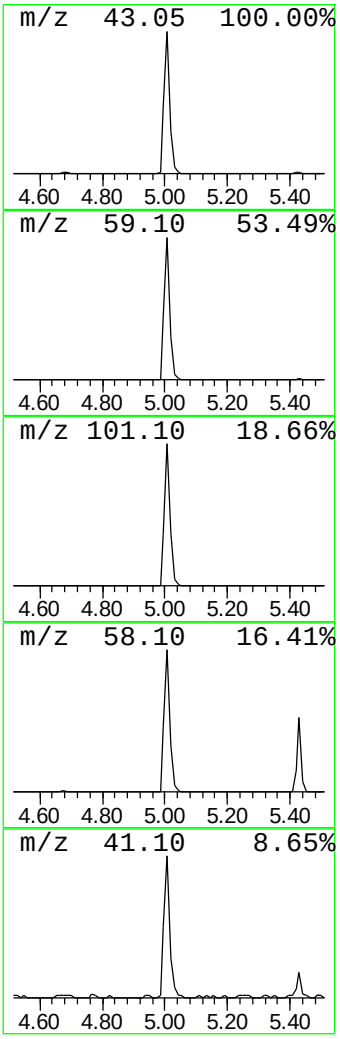
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	9.71 ng	689421	1,4-Dichlorobenzene-d4	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9





Library Search Compound Report

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Operator : SJ/MA
Sample : I2304-07 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SPA-B4(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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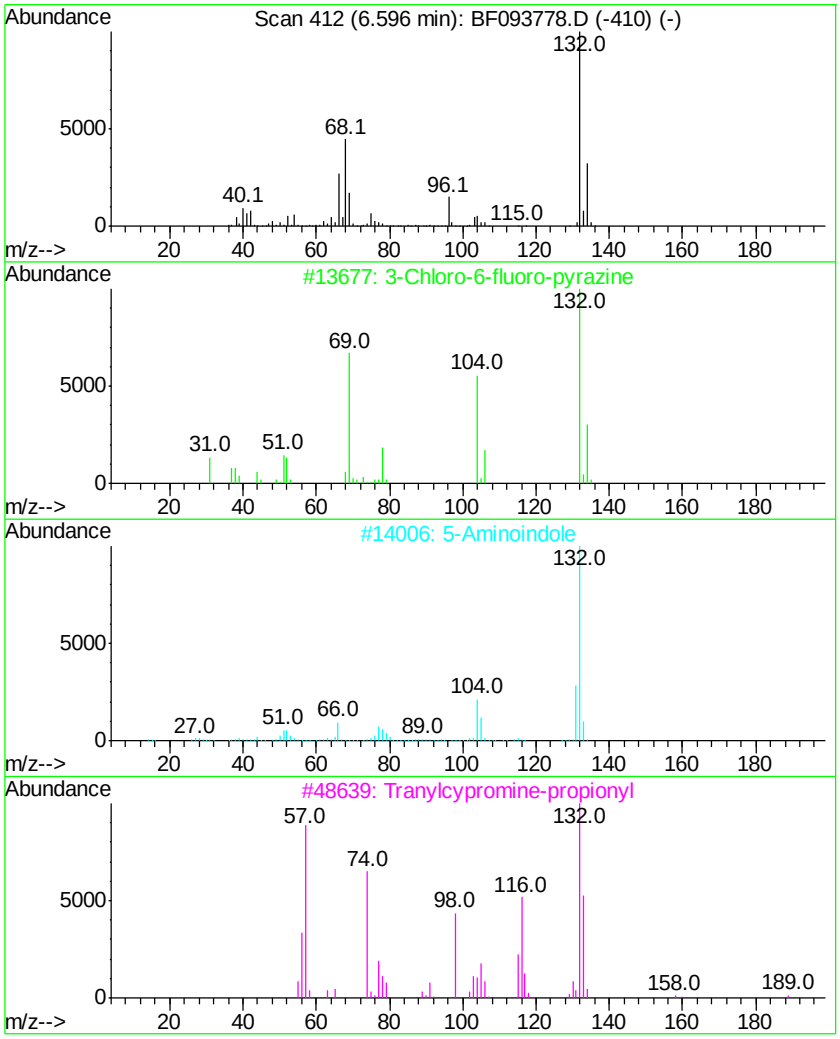
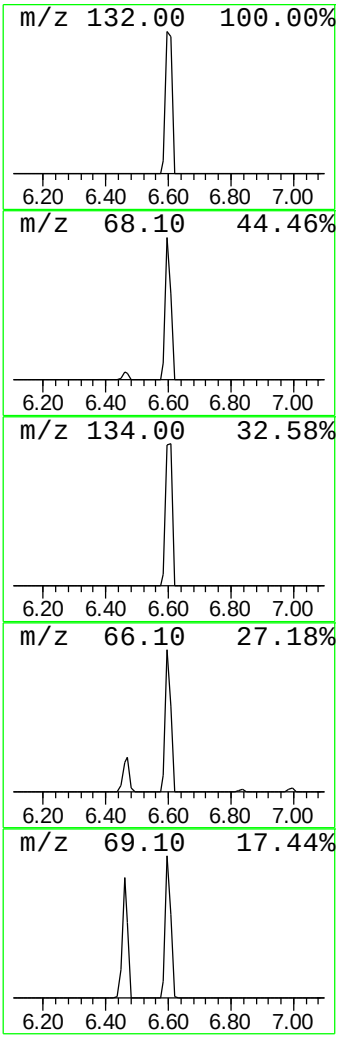
Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	49.80 ng	3535990	1,4-Dichlorobenzene-d4	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF032017\
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Operator : SJ/MA
Sample : I2304-07 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SPA-B4(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
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TIC Library : C:\DATABASE\NIST02.L
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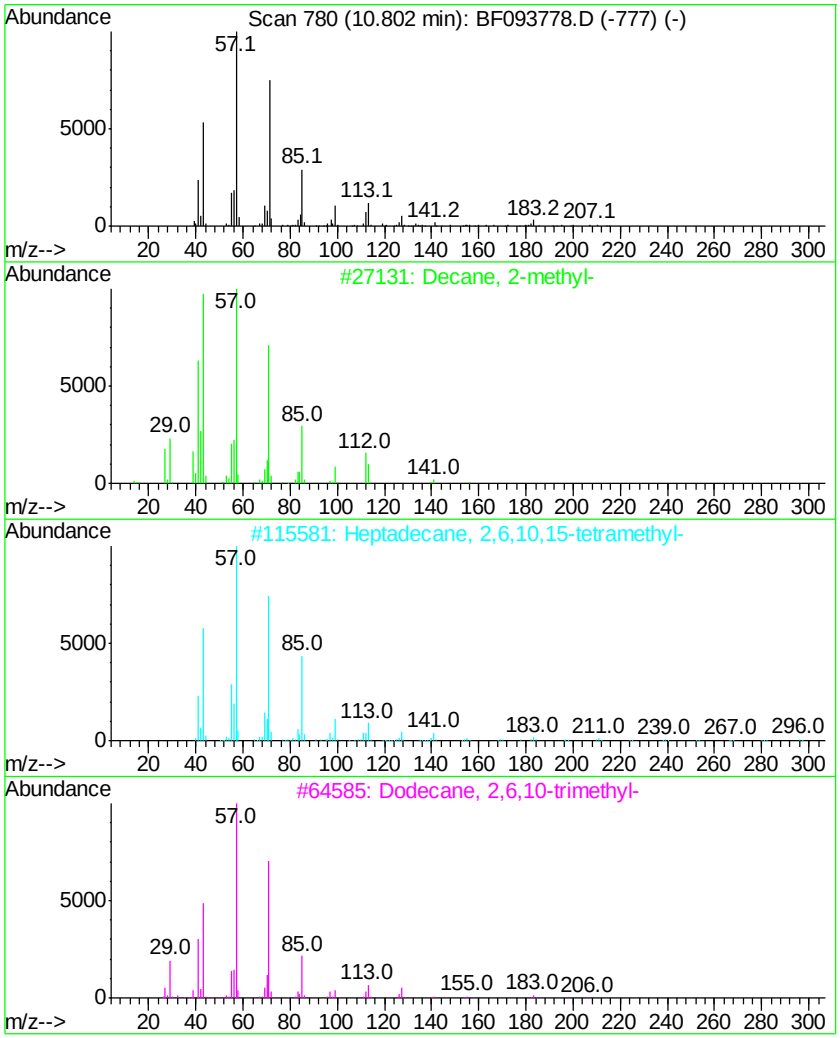
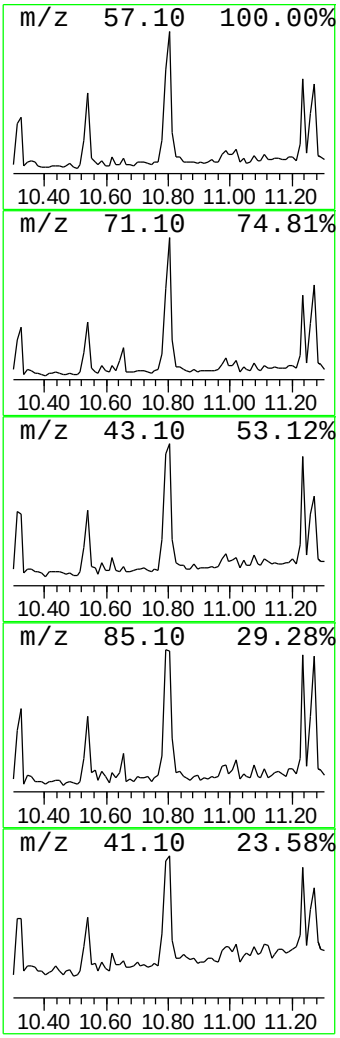
Peak Number 4 Decane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	5.55 ng	447066	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 2-methyl-	156	C11H24	006975-98-0	86
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	83
3	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	83
4	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	80
5	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	80





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Misc :
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Instrument : BNA_F
ClientSampleId : SPA-B4(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
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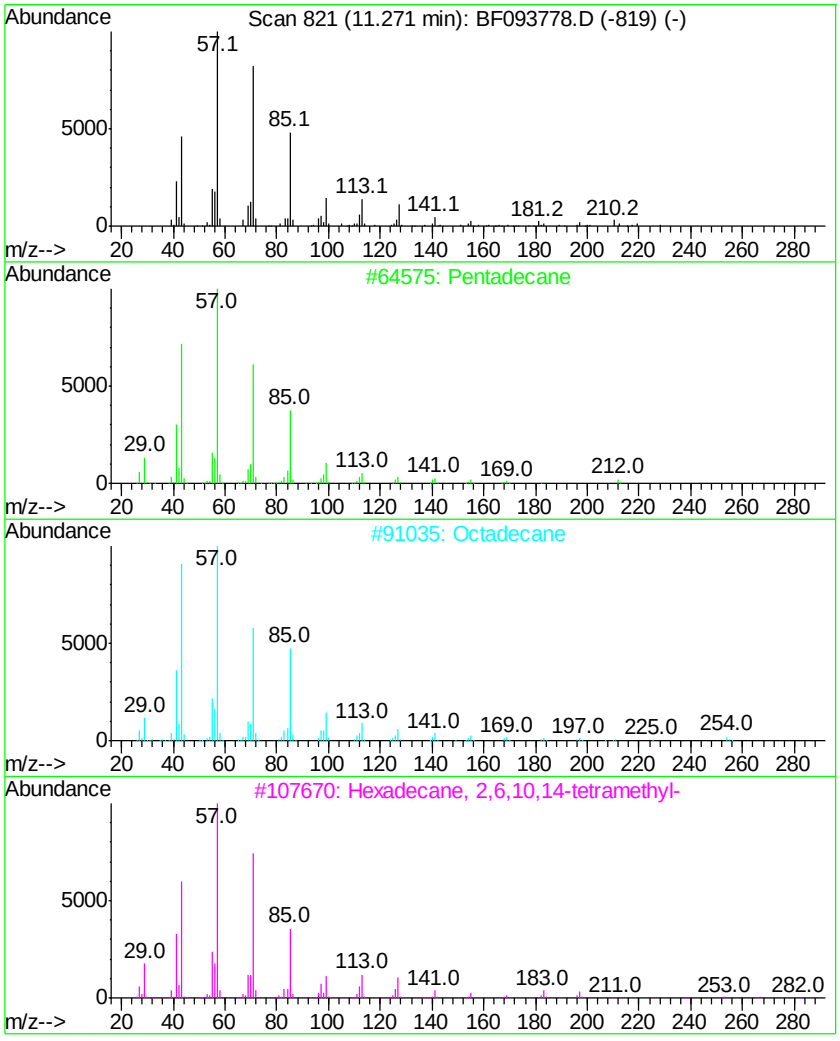
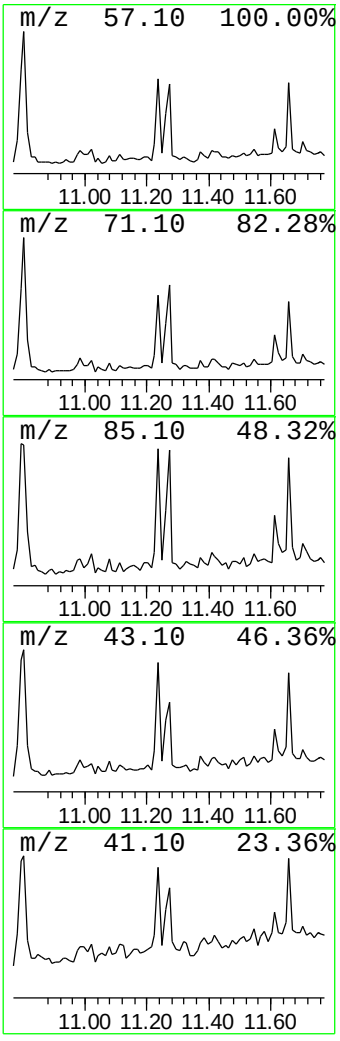
Peak Number 5 Pentadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.27	2.50 ng	201844	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	91
2	Octadecane	254	C18H38	000593-45-3	90
3	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	90
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
5	Octacosane	394	C28H58	000630-02-4	78





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Instrument : BNA_F
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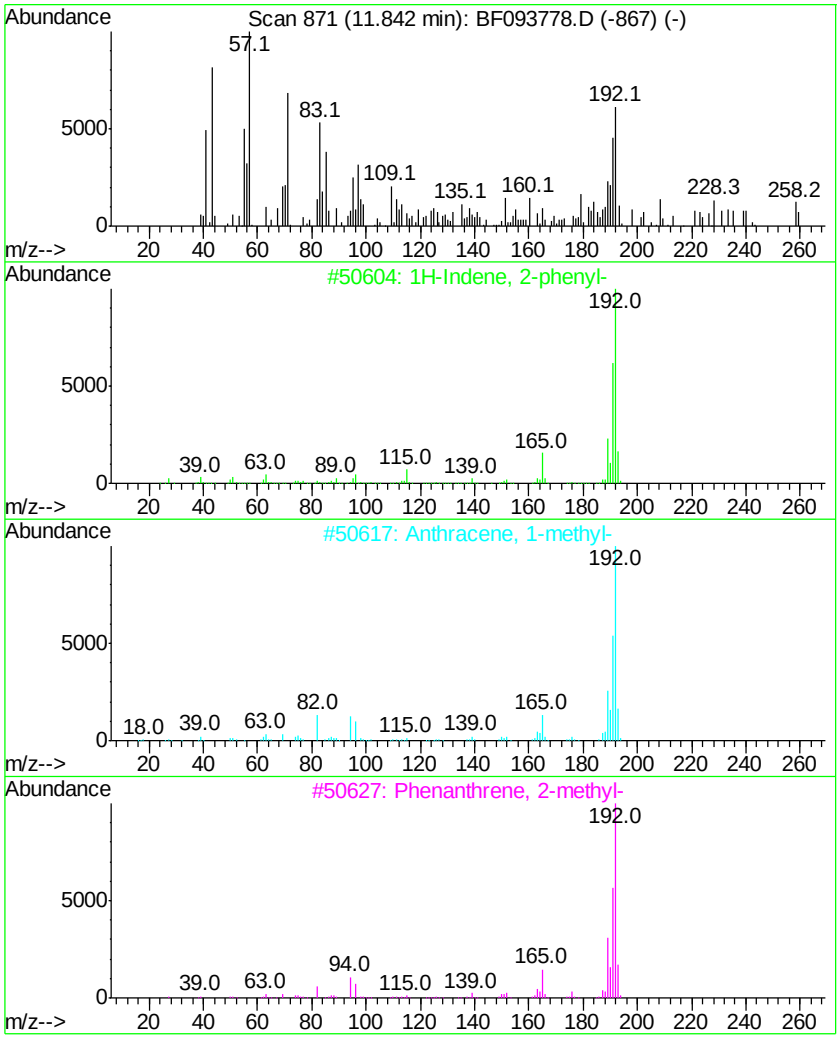
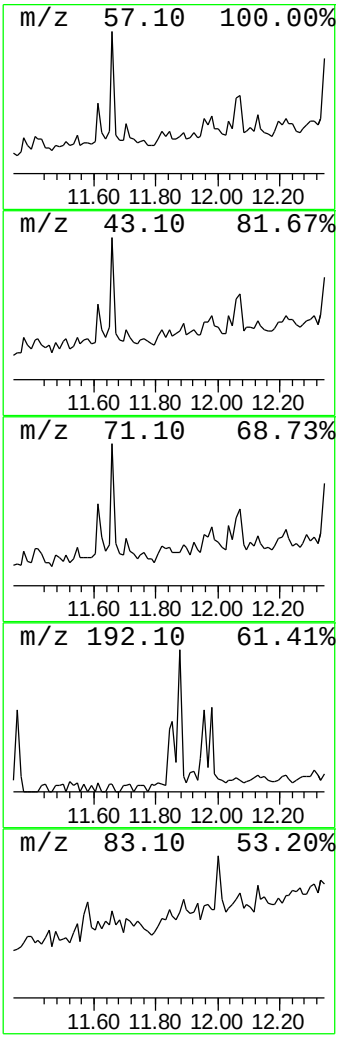
Peak Number 6 unknown11.84 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	2.24 ng	180539	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	38
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	38
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	38
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	30
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	30





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Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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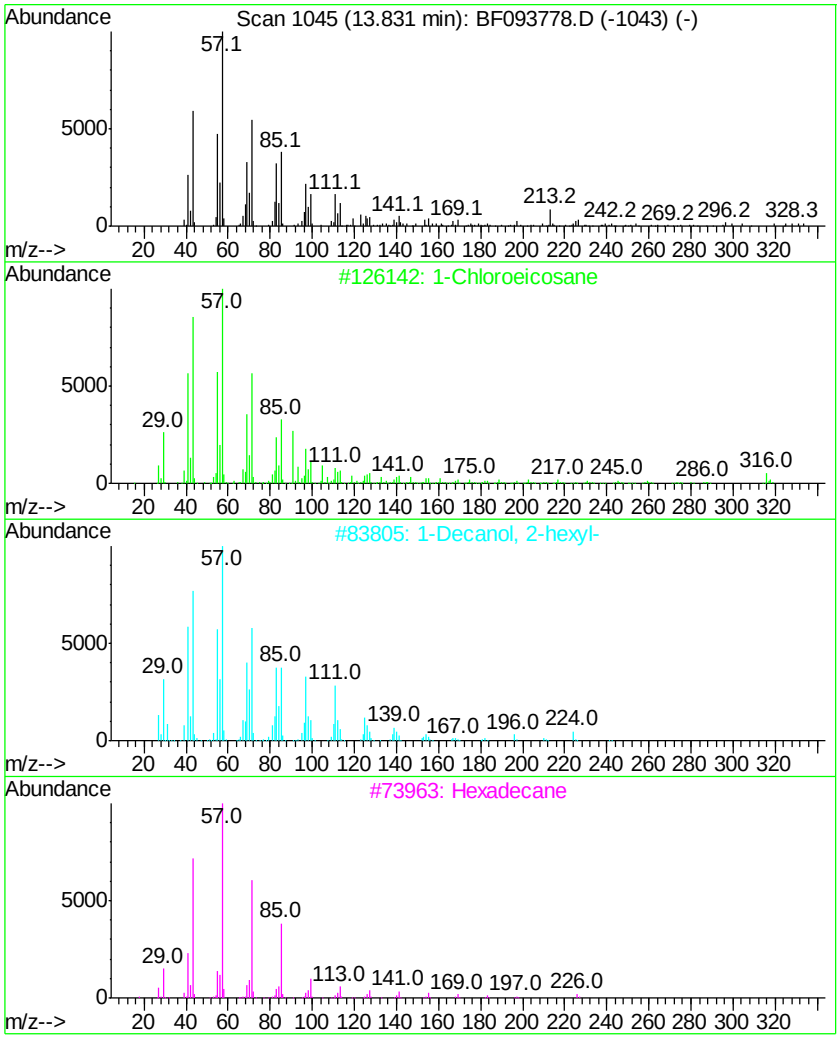
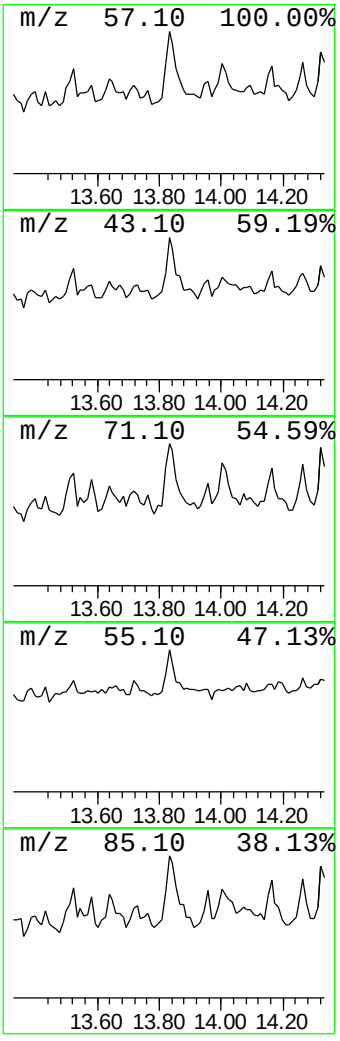
Peak Number 7 1-Chloroeicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	7.13 ng	375225	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Chloroeicosane	316	C20H41Cl	042217-02-7	87
2	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	74
3	Hexadecane	226	C16H34	000544-76-3	70
4	Heptadecane	240	C17H36	000629-78-7	64
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	60





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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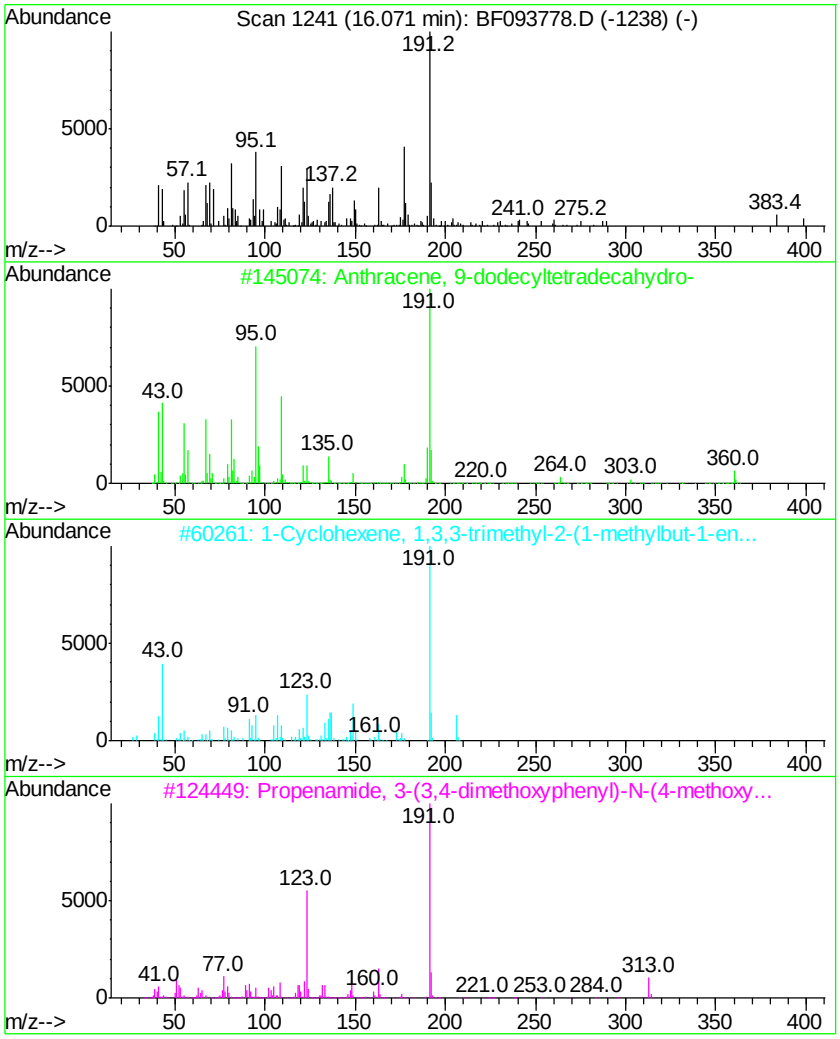
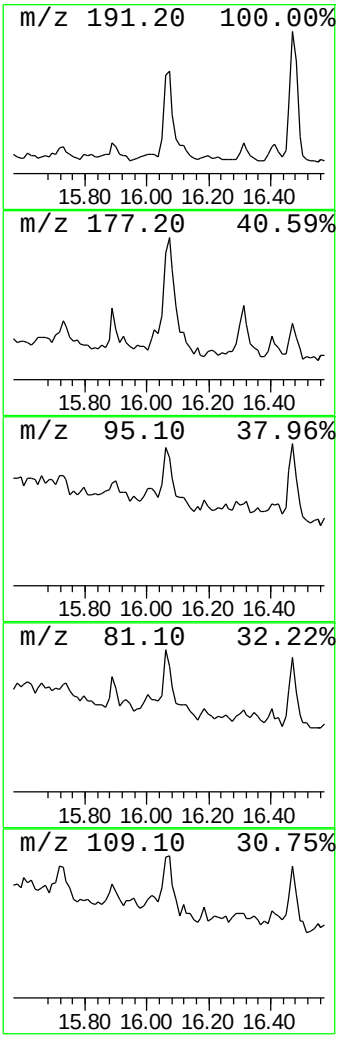
Peak Number 8 unknown16.07 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.07	8.39 ng	428134	Perylene-d12	15.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	43
2	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	38
3	Propenamide, 3-(3,4-dimethoxyphe...	313	C18H19NO4	339165-72-9	35
4	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	32
5	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	32





Data Path : Z:\HPCHEM1\BNA F\DATA\BF032017\
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Operator : SJ/MA
Sample : I2304-07 2X
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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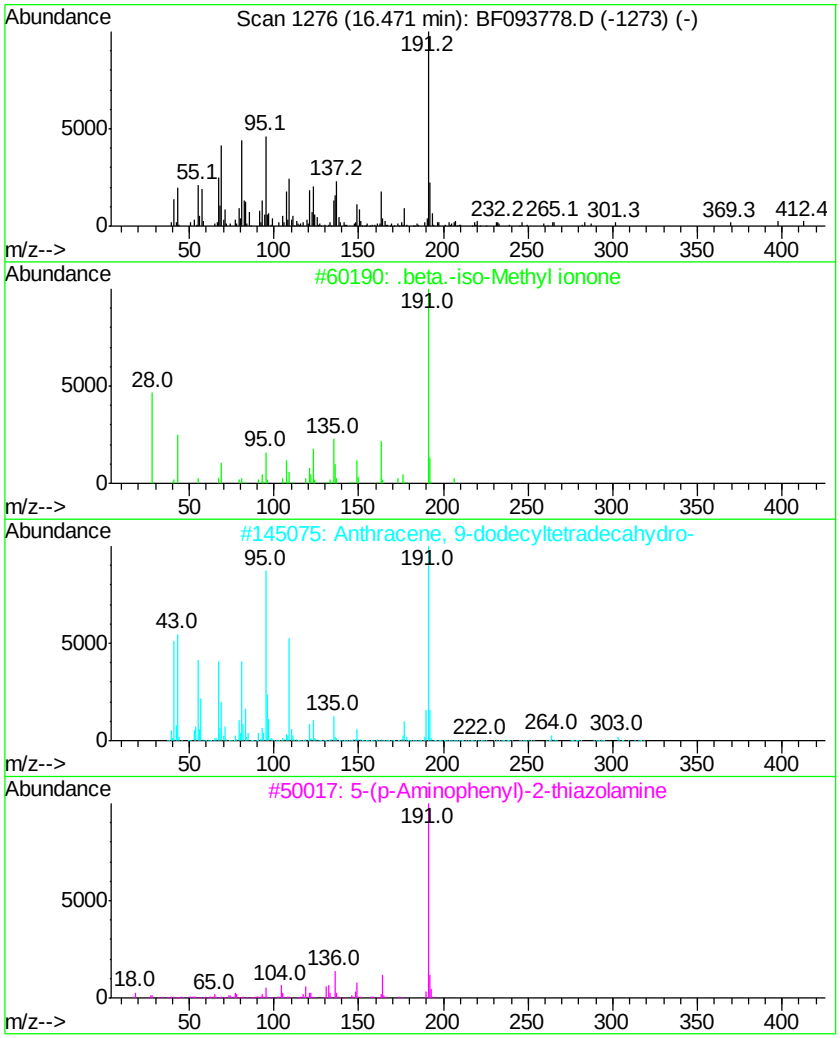
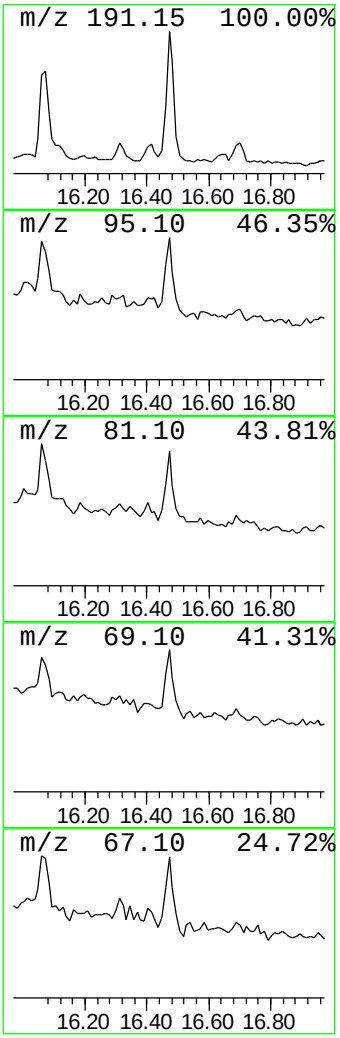
Peak Number 9 .beta.-iso-Methyl ionone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.47	6.98 ng	356127	Perylene-d12	15.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	52
2	Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	40
3	5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	38
4	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	38
5	4-(3H-Imidazo[4,5-b]pyridin-2-yl...	342	C15H18N8S	1000276-08-2	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032017\
Data File : BF093778.D
Acq On : 20 Mar 2017 21:42
Operator : SJ/MA
Sample : I2304-07 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SPA-B4(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.01	9.7	ng	689421	1	6.84	1420220	20.0
unknown6.60	6.60	49.8	ng	3535990	1	6.84	1420220	20.0
Decane, 2-methyl-	10.80	5.5	ng	447066	4	11.35	1612250	20.0
Pentadecane	11.27	2.5	ng	201844	4	11.35	1612250	20.0
unknown11.84	11.84	2.2	ng	180539	4	11.35	1612250	20.0
1-Chloroeicosane	13.83	7.1	ng	375225	5	13.97	1052450	20.0
unknown16.07	16.07	8.4	ng	428134	6	15.39	1020700	20.0
.beta.-iso-Methyl...	16.47	7.0	ng	356127	6	15.39	1020700	20.0