LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089060.D
Acq On : 16 Jul 2016 17:42
Operator : UM/SJ
Sample : H3989-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q7-B6(0-11)C

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-BF063016.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	1.655	3	6	14	rVV	76170	192258	15.41%	1.313%
2	1.770	14	16	34	rVB	769005	1247534	100.00%	8.521%
3	4.798	279	281	285	rBV	102829	142453	11.42%	0.973%
4	5.256	319	321	324	rBV	1194594	1192275	95.57%	8.143%
5	6.319	411	414	417	rBV	1084708	1181251	94.69%	8.068%
6	6.433	422	424	427	rBV	1171747	1223062	98.04%	8.354%
7	6.662	442	444	446	rBV	383396	327455	26.25%	2.237%
8	6.822	455	458	460	rBV	1239666	1015991	81.44%	6.939%
9	7.233	491	494	496	rBV	841645	785186	62.94%	5.363%
10	7.702	532	535	539	rVB	10915	15409	1.24%	0.105%
11	7.953	555	557	559	rBV	463379	426256	34.17%	2.911%
12	8.387	593	595	599	rBV2	8208	13695	1.10%	0.094%
13	9.027	649	651	654	rVB	1213774	1115157	89.39%	7.617%
14	9.119	656	659	662	rBV2	11943	24063	1.93%	0.164%
15	9.290	671	674	676	rBV	9505	13916	1.12%	0.095%
16	9.359	679	680	682	rBV2	11478	15461	1.24%	0.106%
17	9.428	684	686	688	rBV	280065	232272	18.62%	1.586%
18	9.565	696	698	701	rBV	11429	12898	1.03%	0.088%
19	9.656	704	706	707	rVB	16824	16556	1.33%	0.113%
20	9.702	708	710	712	rVV	474213	403268	32.33%	2.754%
21	9.736	712	713	715	rVB	23758	17297	1.39%	0.118%
22	9.908	724	728	729	rBV	19735	20477	1.64%	0.140%
23	10.113	741	746	748	rBV	9486	18989	1.52%	0.130%
24	10.148	748	749	751	rVV	28181	25611	2.05%	0.175%
25	10.250	755	758	761	rVB	14285	26222	2.10%	0.179%
26	10.365	766	768	770	rVB	19152	27798	2.23%	0.190%
27	10.490	777	779	781	rBV	627720	584122	46.82%	3.990%
28	10.628	789	791	794	rVB	36577	71745	5.75%	0.490%
29	10.948	816	819	821	rBV3	7071	13394	1.07%	0.091%
30	11.073	828	830	831	rBV	43350	50453	4.04%	0.345%
31	11.176	837	839	843	rBV2	345563	510541	40.92%	3.487%
32	11.256	843	846	847	rVB	51796	55101	4.42%	0.376%
33	11.416	857	860	861	rBV2	21263	20566	1.65%	0.140%
34	11.496	865	867	870	rBV2	36522	46466	3.72%	0.317%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089060.D
Acq On : 16 Jul 2016 17:42
Operator : UM/SJ
Sample : H3989-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q7-B6(0-11)C

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-BF063016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.553	870	872	874	rVB3	10669	14464	1.16%	0.099%
36	11.588	874	875	877	rBV2	17035	22074	1.77%	0.151%
37	11.679	881	883	885	rBV2	25083	43575	3.49%	0.298%
38	11.759	888	890	891	rVB	15193	14660	1.18%	0.100%
39	11.793	891	893	898	rBV2	49895	96004	7.70%	0.656%
40	11.908	898	903	905	rBV3	26201	73785	5.91%	0.504%
41	11.999	905	911	914	rBV5	55567	120800	9.68%	0.825%
42	12.079	915	918	919	rBV3	14856	32254	2.59%	0.220%
43	12.102	919	920	923	rBV3	31110	50577	4.05%	0.345%
44	12.182	923	927	928	rVB3	22287	40337	3.23%	0.276%
45	12.228	929	931	933	rBV	48531	76030	6.09%	0.519%
46	12.319	937	939	940	rBV2	15939	17343	1.39%	0.118%
47	12.388	943	945	947	rBV	384318	305871	24.52%	2.089%
48	12.445	947	950	952	rVB4	25902	44984	3.61%	0.307%
49	12.491	952	954	956	rBV2	25004	58172	4.66%	0.397%
50	12.616	962	965	968	rBV	288869	397684	31.88%	2.716%
51	12.765	976	978	981	rBV	778532	812536	65.13%	5.550%
52	12.948	992	994	996	rVB	80405	82406	6.61%	0.563%
53	13.051	1001	1003	1006	rBV3	47710	112811	9.04%	0.771%
54	13.211	1015	1017	1019	rBV	78138	75216	6.03%	0.514%
55	13.817	1067	1070	1074	rBV2	369026	734627	58.89%	5.018%
56	14.617	1138	1140	1143	rBV3	199055	329506	26.41%	2.251%

Sum of corrected areas: 14640914

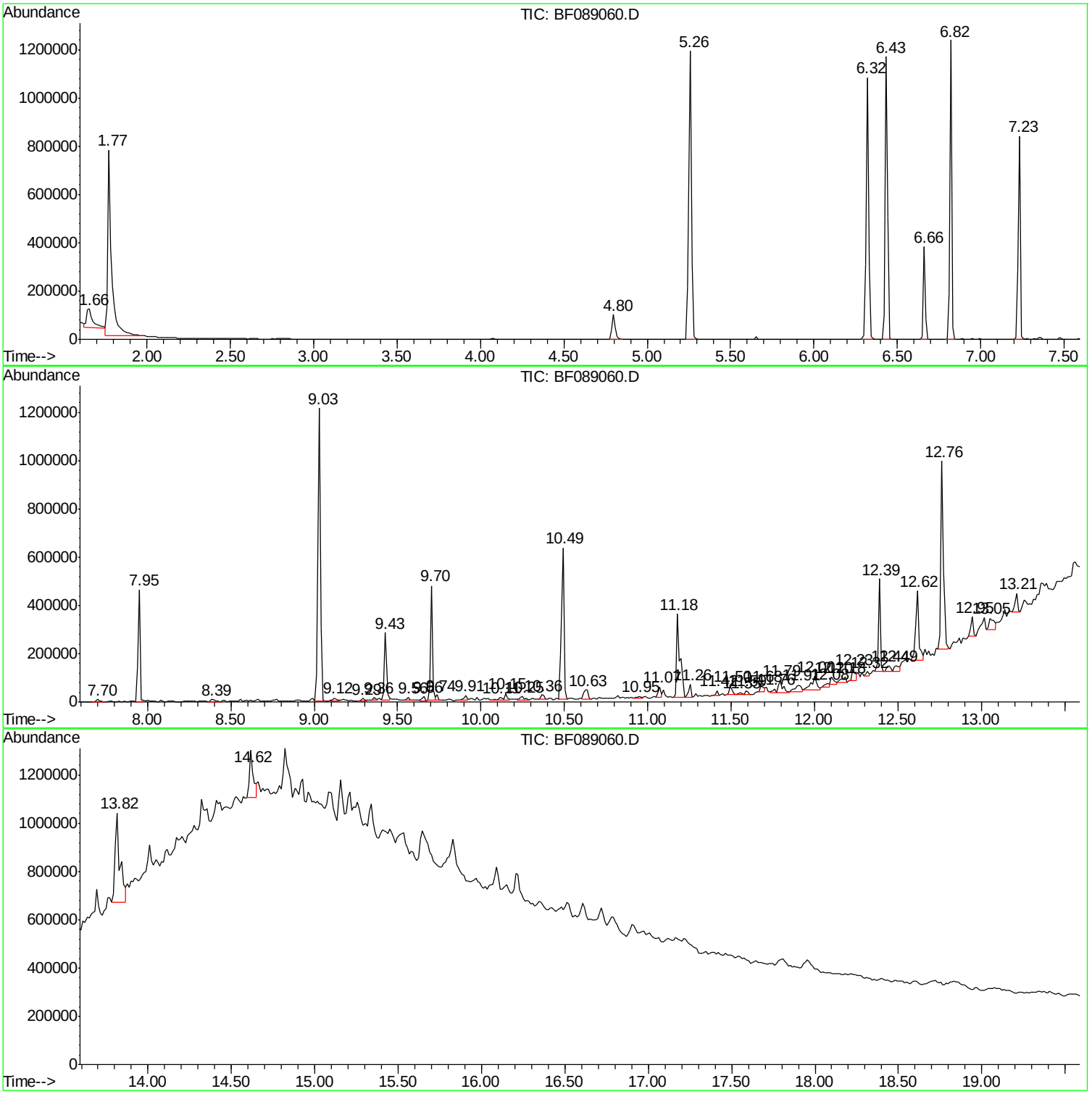
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089060.D
Acq On : 16 Jul 2016 17:42
Operator : UM/SJ
Sample : H3989-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
Q7-B6(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089060.D
Acq On : 16 Jul 2016 17:42
Operator : UM/SJ
Sample : H3989-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q7-B6(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

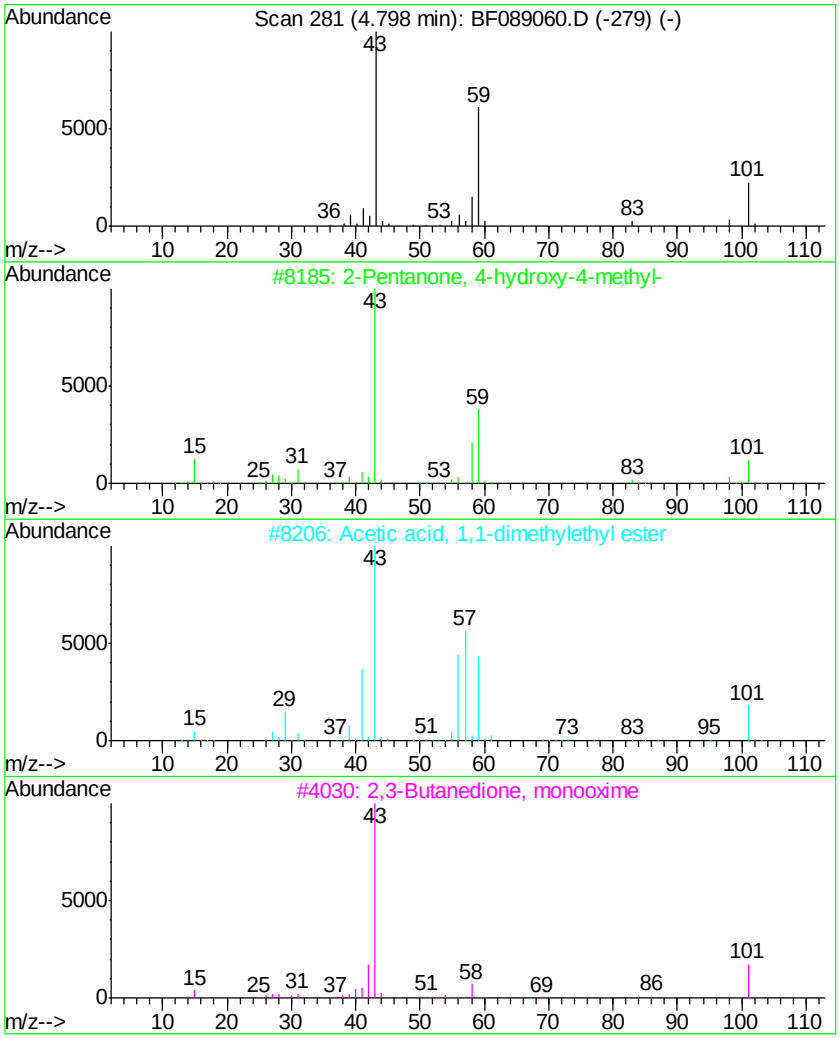
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

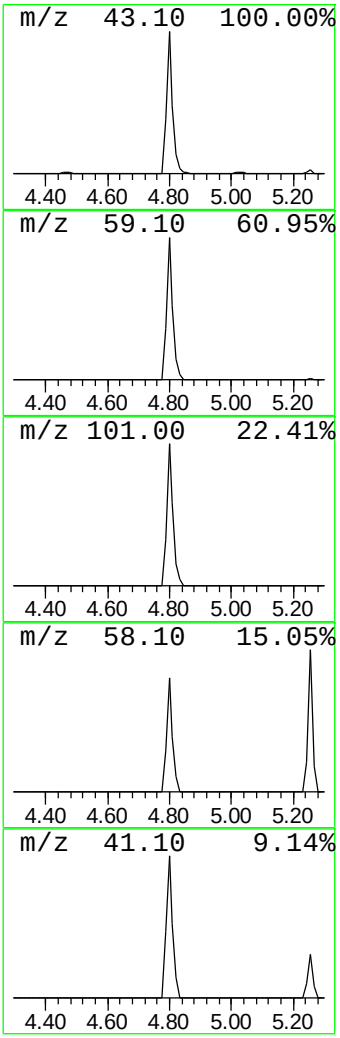
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	8.70 ng	142453	1,4-Dichlorobenzene-d4	6.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089060.D
Acq On : 16 Jul 2016 17:42
Operator : UM/SJ
Sample : H3989-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q7-B6(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

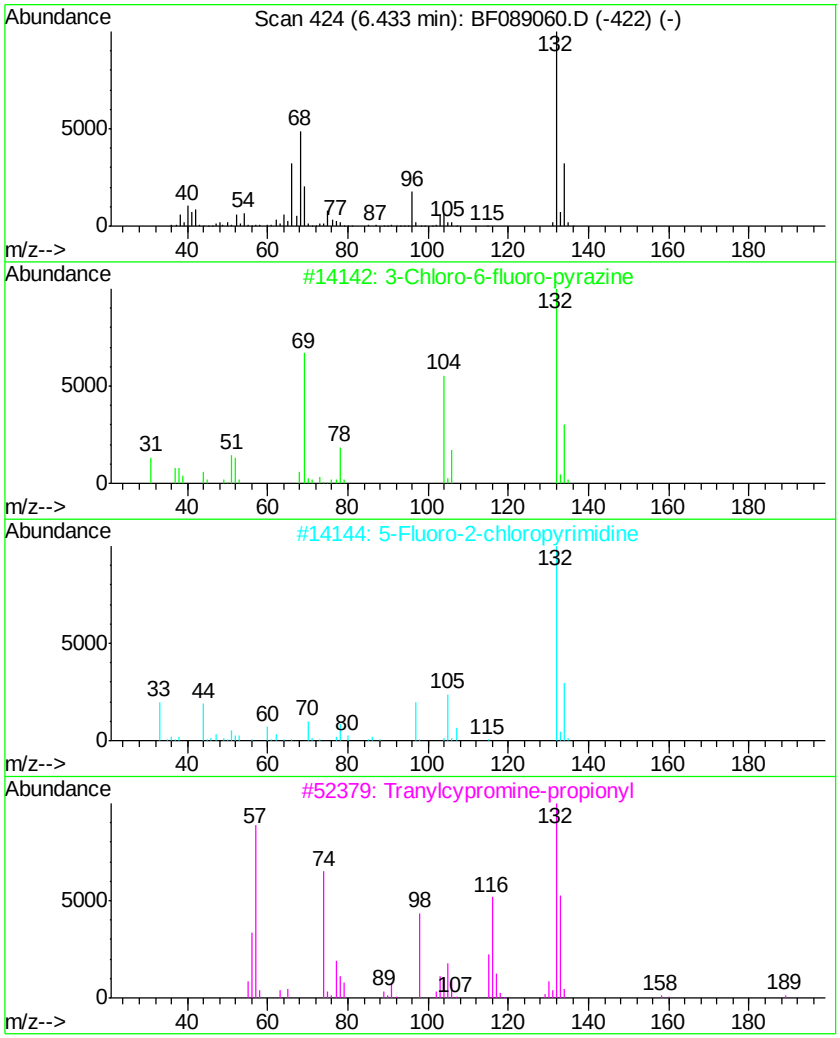
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

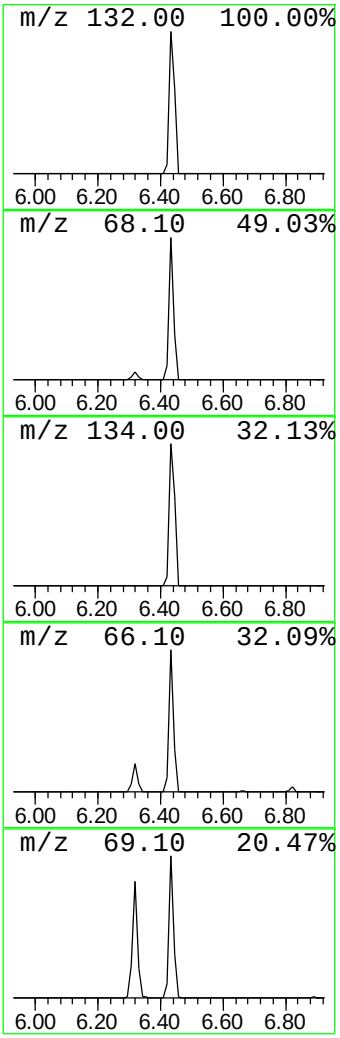
****

Peak Number 4 unknown6.43 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.43	74.70 ng	1223060	1,4-Dichlorobenzene-d4	6.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089060.D
Acq On : 16 Jul 2016 17:42
Operator : UM/SJ
Sample : H3989-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q7-B6(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

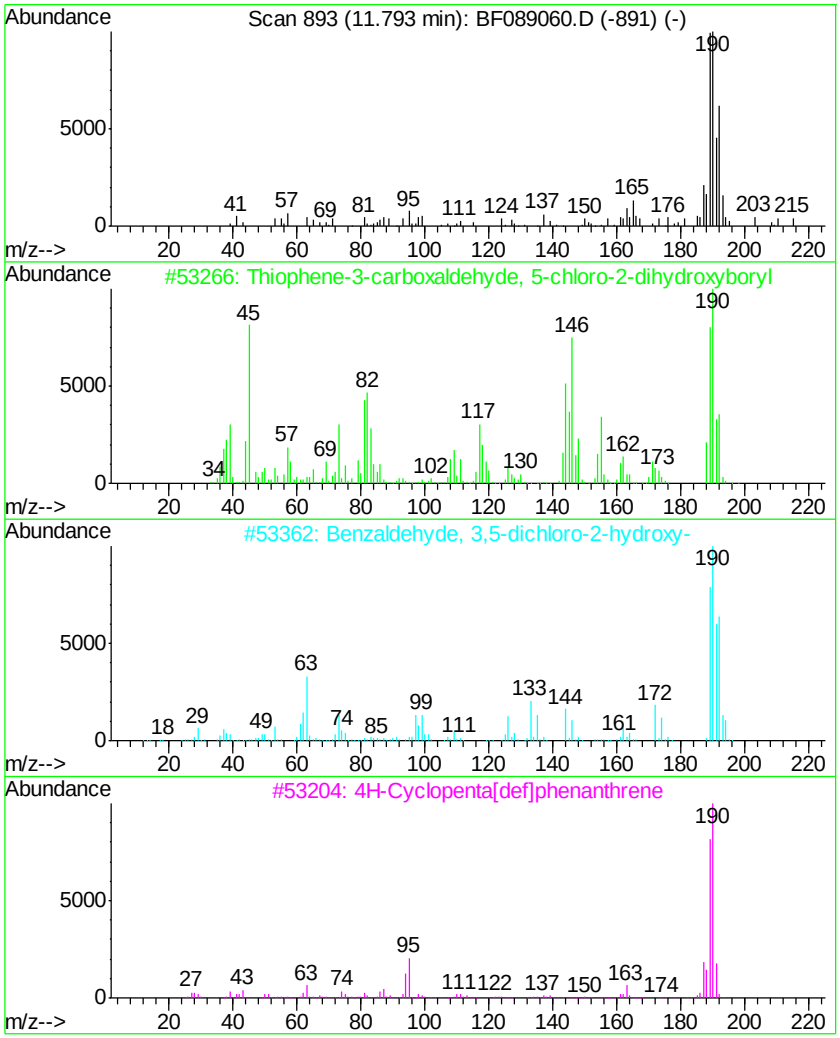
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

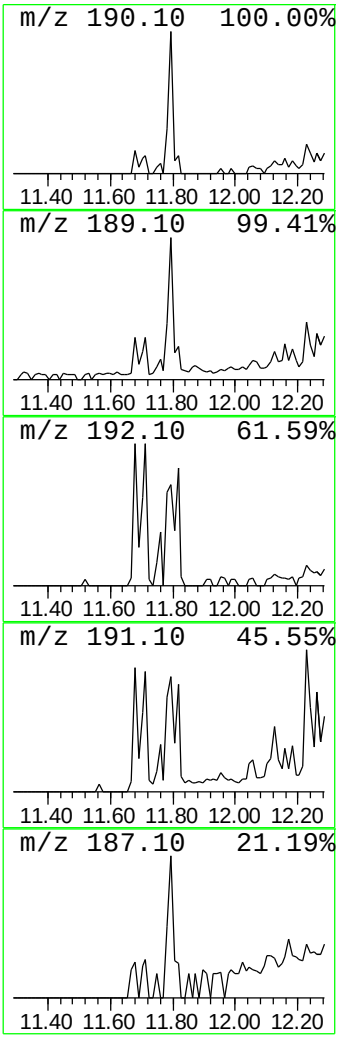
****

Peak Number 7 Thiophene-3-carboxaldehyde,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	3.76 ng	96004	Phenanthrene-d10	11.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	59
2	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	53
3	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	49
4	Cyclohexanone, 2-(2-furanylmethy...	190	C12H14O2	056053-07-7	27
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	20





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089060.D
Acq On : 16 Jul 2016 17:42
Operator : UM/SJ
Sample : H3989-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q7-B6(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

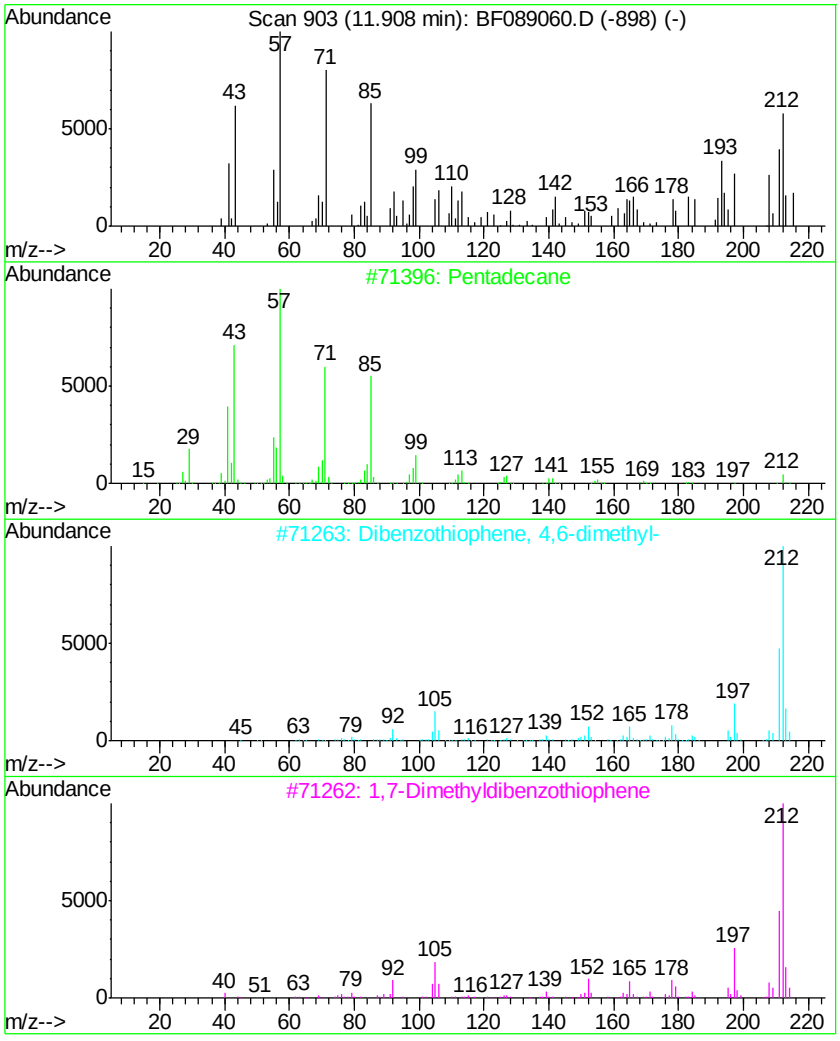
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

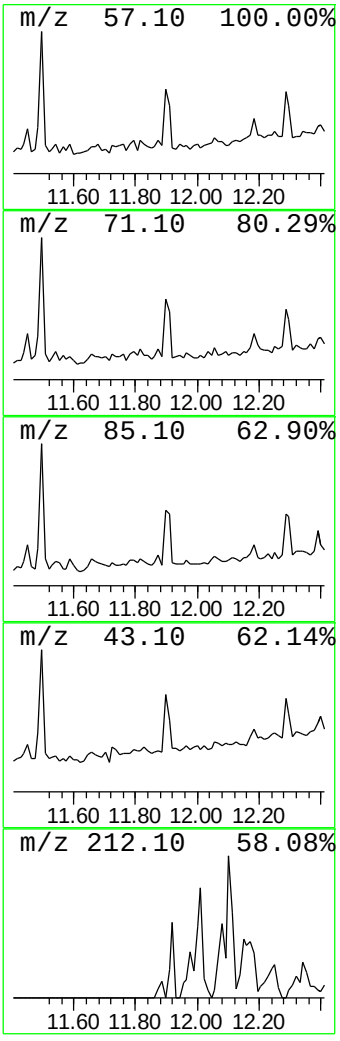
****

Peak Number 8 unknown11.91 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	2.89 ng	73785	Phenanthrene-d10	11.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	43
2	Dibenzothiophene, 4,6-dimethyl-	212	C14H12S	001207-12-1	38
3	1,7-Dimethyldibenzothiophene	212	C14H12S	089816-53-5	35
4	2,7-Dimethyldibenzothiophene	212	C14H12S	031317-19-8	30
5	Decane, 1-iodo-	268	C10H21I	002050-77-3	27





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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q7-B6(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

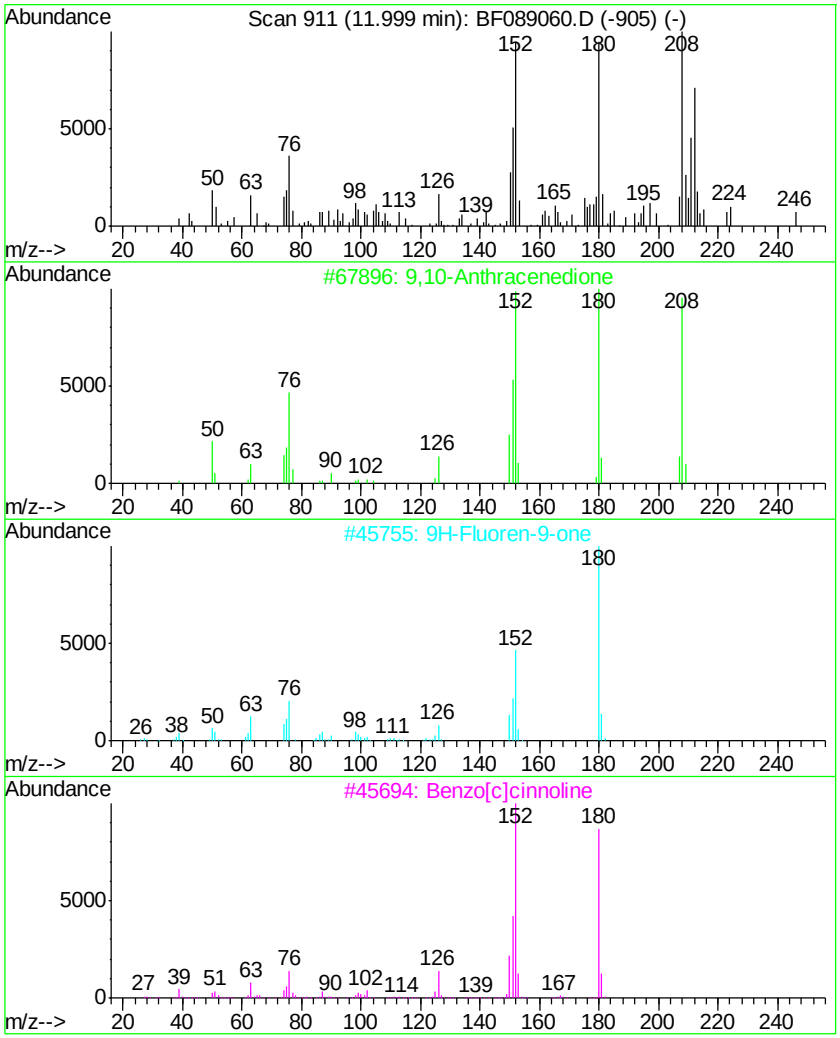
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

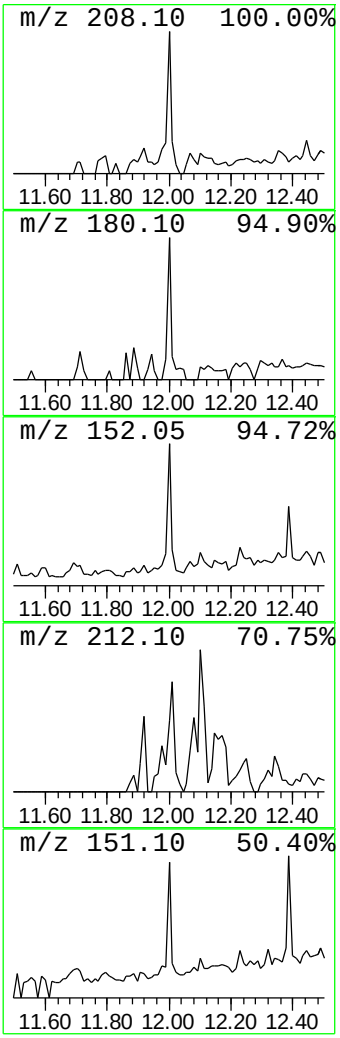
****

Peak Number 9 9,10-Anthracenedione Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	4.73 ng	120800	Phenanthrene-d10	11.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione	208	C14H8O2	000084-65-1	97
2	9H-Fluoren-9-one	180	C13H8O	000486-25-9	95
3	Benzo[c]cinnoline	180	C12H8N2	000230-17-1	89
4	1H-Phenalen-1-one	180	C13H8O	000548-39-0	45
5	Benzo[h]cinnoline	180	C12H8N2	000230-31-9	41





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Sample : H3989-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q7-B6(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

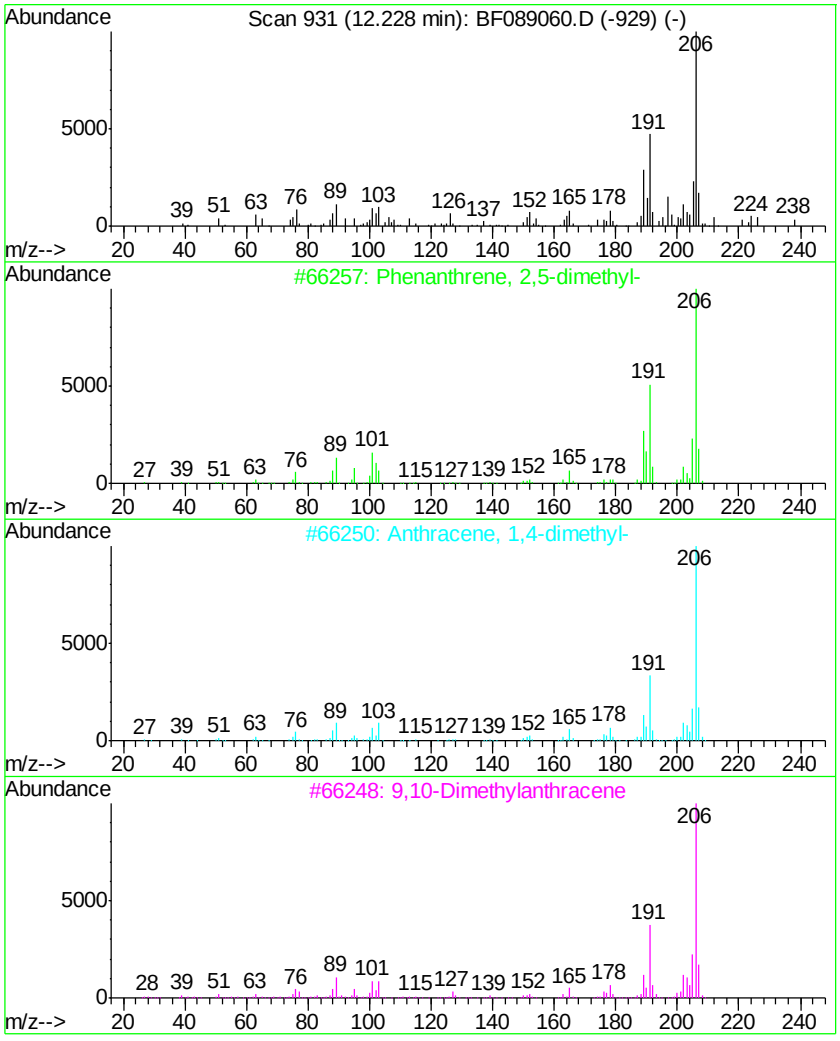
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

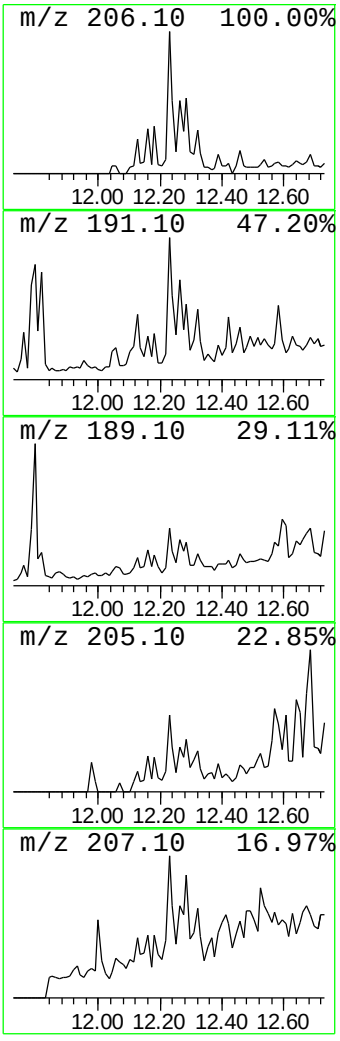
****

Peak Number 10 Phenanthrene, 2,5-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.23	2.98 ng	76030	Phenanthrene-d10	11.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	96
2	Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	94
3	9,10-Dimethylanthracene	206	C16H14	000781-43-1	92
4	di-p-Tolylacetylene	206	C16H14	002789-88-0	91
5	Phenanthrene, 2,7-dimethyl-	206	C16H14	001576-69-8	89





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089060.D
Acq On : 16 Jul 2016 17:42
Operator : UM/SJ
Sample : H3989-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q7-B6(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

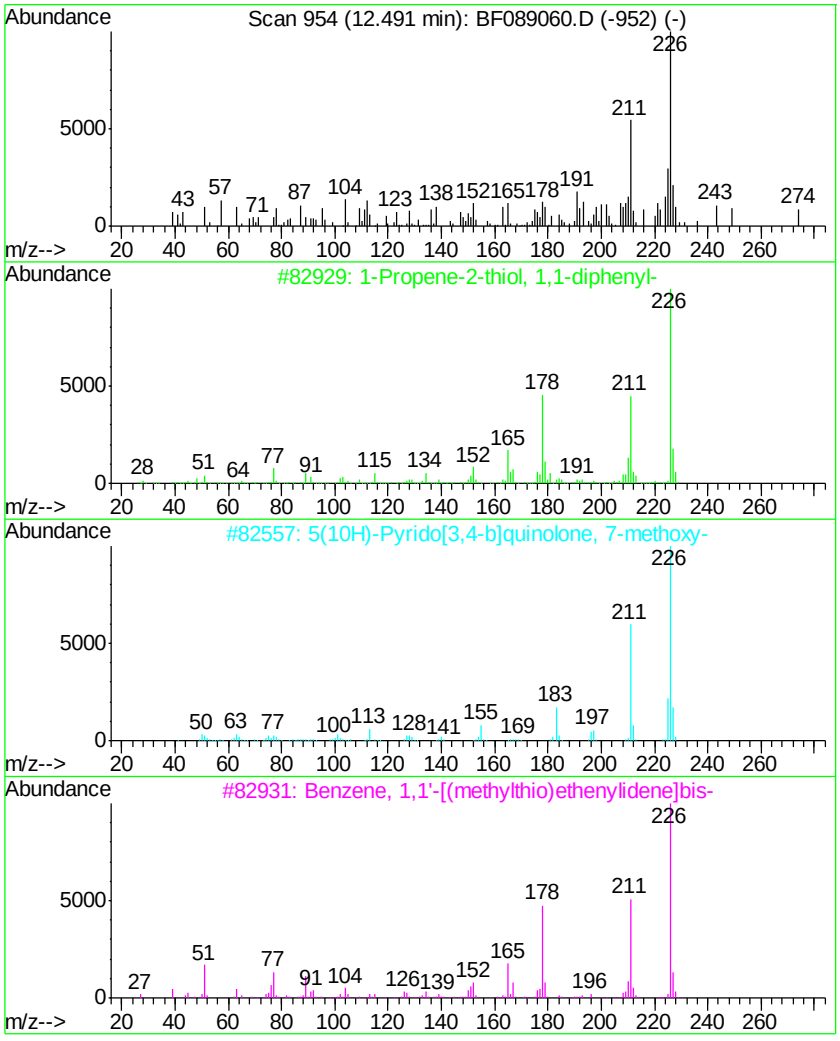
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

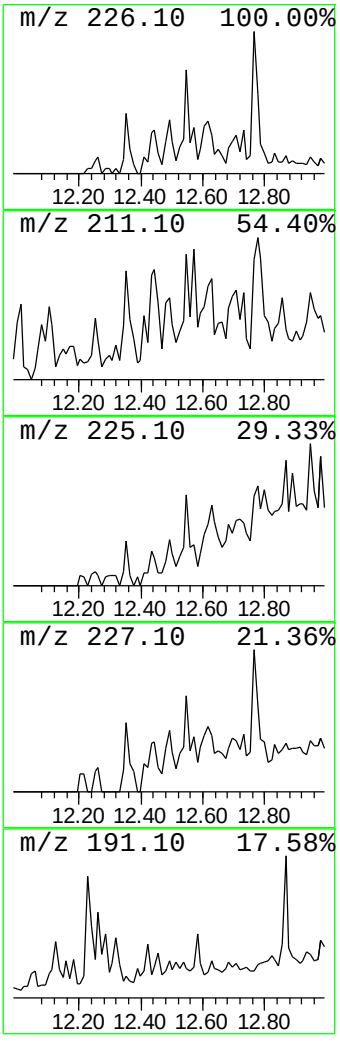
****

Peak Number 11 1-Propene-2-thiol, 1,1-diph... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.49	2.28 ng	58172	Phenanthrene-d10	11.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene-2-thiol, 1,1-diphenyl-	226	C15H14S	074630-83-4	70
2	5(10H)-Pyrido[3,4-b]quinolone, 7...	226	C13H10N2O2	1000256-99-5	58
3	Benzene, 1,1'-[(methylthio)ethen...	226	C15H14S	015096-10-3	58
4	N,N-Dimethylindoaniline	226	C14H14N2O	002150-58-5	50
5	Anthracene, 1,8-diethynyl-	226	C18H10	078053-58-4	49





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089060.D
Acq On : 16 Jul 2016 17:42
Operator : UM/SJ
Sample : H3989-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q7-B6(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

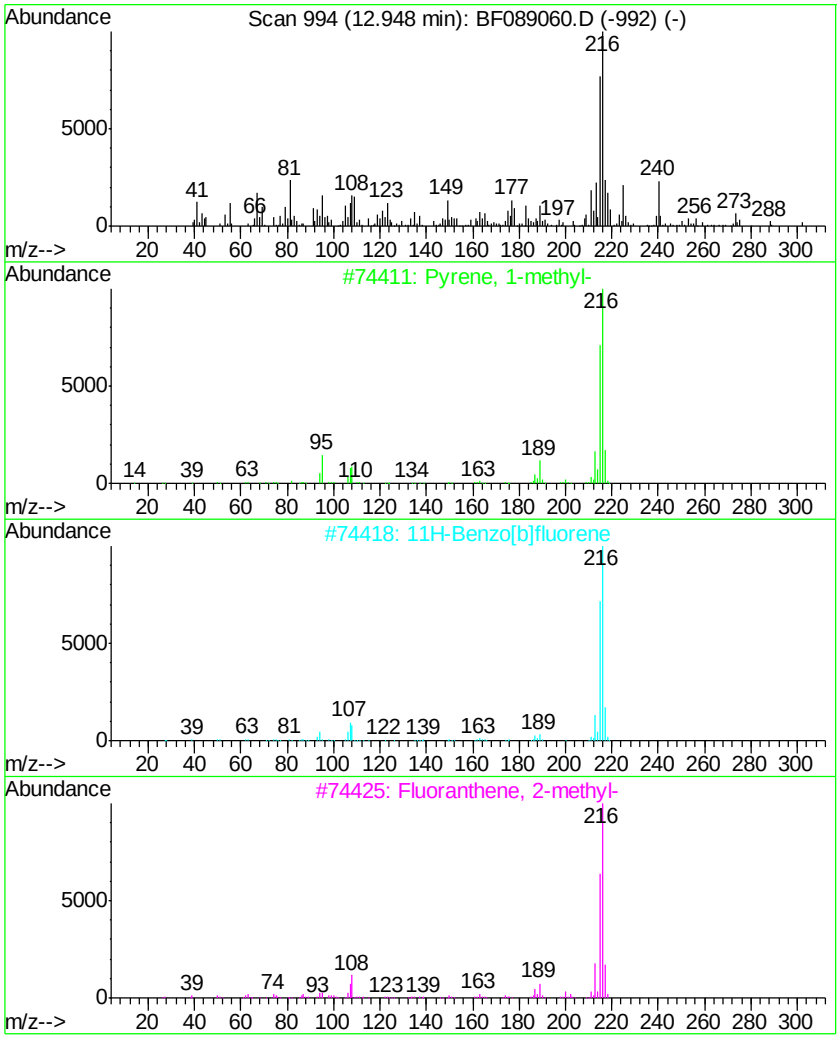
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

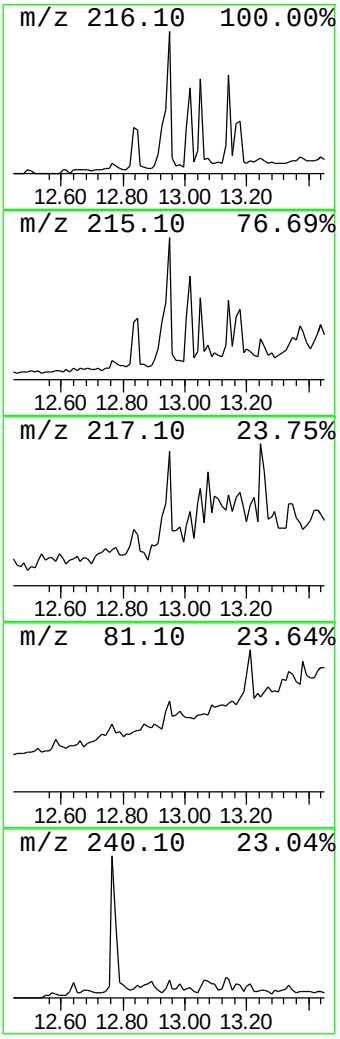
****

Peak Number 12 Pyrene, 1-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.95	2.24 ng	82406	Chrysene-d12	13.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	89
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	76
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	70
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	68
5	1,3,5-Triazine-2,4,6-triamine, N...	216	C10H12N6	046731-79-7	58





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Data File : BF089060.D
Acq On : 16 Jul 2016 17:42
Operator : UM/SJ
Sample : H3989-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q7-B6(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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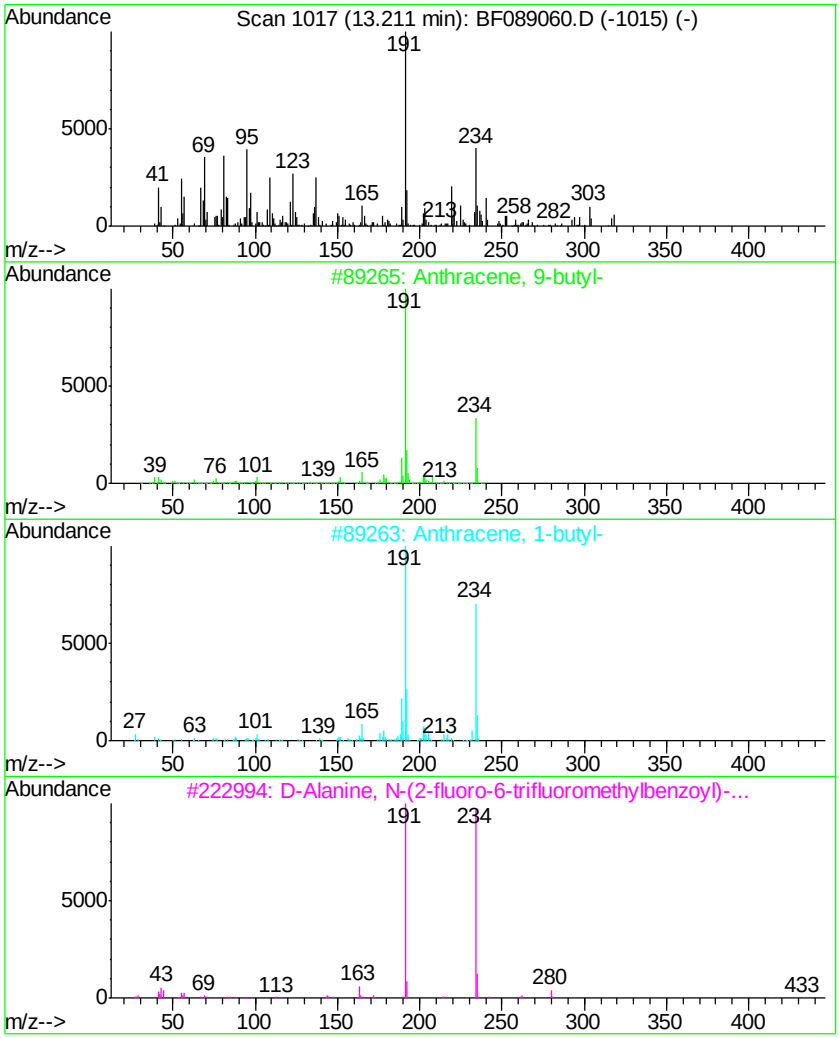
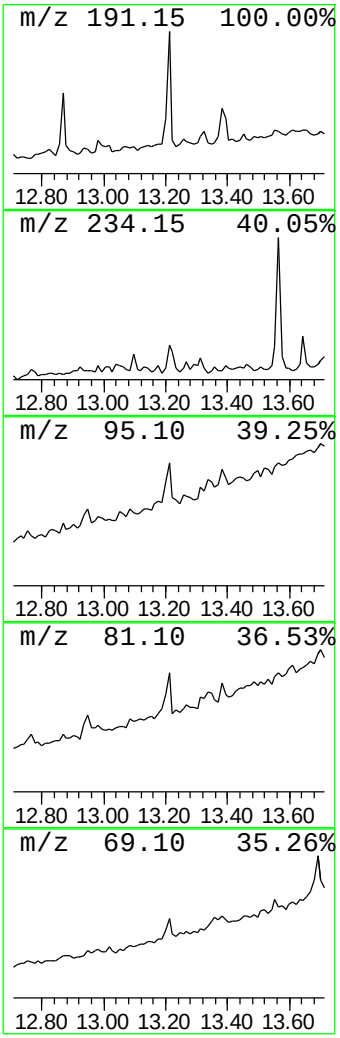
Peak Number 14 unknown13.21 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.21	2.05 ng	75216	Chrysene-d12	13.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 9-butyl-	234	C18H18	001498-69-7	45
2	Anthracene, 1-butyl-	234	C18H18	1000156-51-7	43
3	D-Alanine, N-(2-fluoro-6-trifluo...	433	C22H31F4NO3	1000348-37-7	38
4	dl-9-Cyano-2-oxo-cis-decalin sem...	234	C12H18N4O	002740-39-8	38
5	2-Allyl-1,4-dimethoxy-3-vinyloxy...	234	C14H18O3	1000188-16-6	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089060.D
Acq On : 16 Jul 2016 17:42
Operator : UM/SJ
Sample : H3989-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q7-B6(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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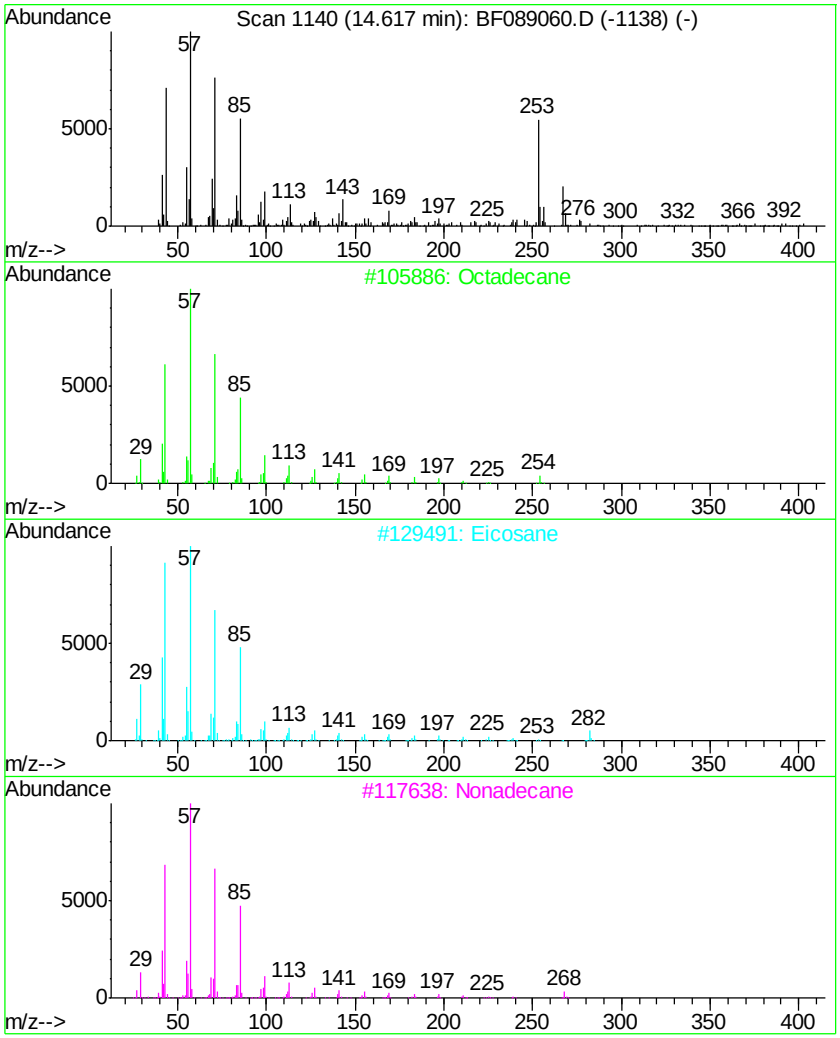
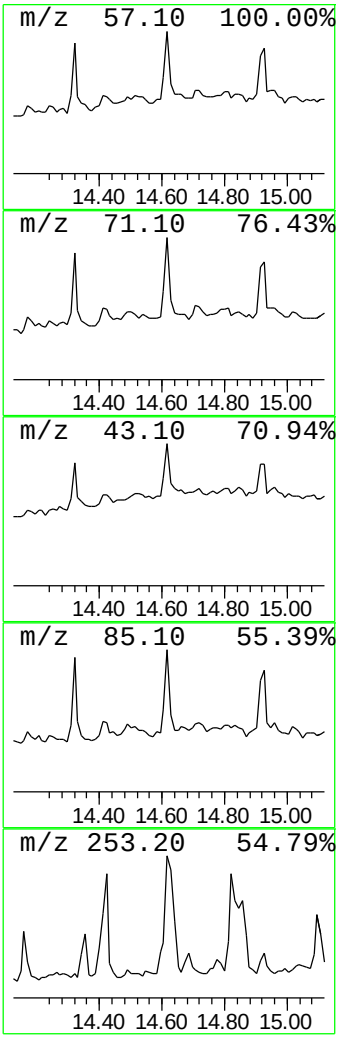
Peak Number 15 Octadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	20.00 ng	329506	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	78
2	Eicosane	282	C20H42	000112-95-8	70
3	Nonadecane	268	C19H40	000629-92-5	70
4	Hexadecane	226	C16H34	000544-76-3	55
5	Octadecane, 2-methyl-	268	C19H40	001560-88-9	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071616\
Data File : BF089060.D
Acq On : 16 Jul 2016 17:42
Operator : UM/SJ
Sample : H3989-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q7-B6(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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...	4.80	8.7	ng	142453	1	6.66	327455	20.0
unknown6.43	6.43	74.7	ng	1223060	1	6.66	327455	20.0
Thiophene-3-carbo...	11.79	3.8	ng	96004	4	11.18	510541	20.0
unknown11.91	11.91	2.9	ng	73785	4	11.18	510541	20.0
9,10-Anthracenedione	12.00	4.7	ng	120800	4	11.18	510541	20.0
Phenanthrene, 2,5...	12.23	3.0	ng	76030	4	11.18	510541	20.0
1-Propene-2-thiol...	12.49	2.3	ng	58172	4	11.18	510541	20.0
Pyrene, 1-methyl-	12.95	2.2	ng	82406	5	13.82	734627	20.0
unknown13.21	13.21	2.0	ng	75216	5	13.82	734627	20.0
Octadecane	14.62	20.0	ng	329506	6	15.21	329506	20.0