LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110116\
Data File : BF090964.D
Acq On : 1 Nov 2016 21:22
Operator : UM/SJ
Sample : H5463-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5(0-2)

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-BF102616.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	4.899	243	246	256	rBV	689626	1025603	20.87%	2.033%
2	5.333	281	284	287	rBV	3743583	4082606	83.06%	8.094%
3	6.384	373	376	378	rBV	3946539	4614189	93.87%	9.148%
4	6.510	384	387	389	rBV	3731789	4880774	99.30%	9.677%
5	6.739	404	407	409	rBV	948711	1065876	21.68%	2.113%
6	6.887	418	420	423	rBV	2790849	3187105	64.84%	6.319%
7	7.299	454	456	459	rBV	2100444	2653447	53.98%	5.261%
8	8.019	517	519	525	rBV	1475196	1762374	35.85%	3.494%
9	9.105	611	614	616	rBV	4747895	4915323	100.00%	9.745%
10	9.185	619	621	627	rVB3	32137	63247	1.29%	0.125%
11	9.436	640	643	644	rBV	61213	62915	1.28%	0.125%
12	9.493	646	648	651	rVV	648151	793509	16.14%	1.573%
13	9.550	651	653	658	rVB2	27814	52014	1.06%	0.103%
14	9.630	658	660	663	rBV	65000	81362	1.66%	0.161%
15	9.722	666	668	670	rVB	67450	79432	1.62%	0.157%
16	9.779	670	673	674	rBV	1566939	1801729	36.66%	3.572%
17	9.802	674	675	678	rVB	47328	56784	1.16%	0.113%
18	9.973	689	690	692	rBV2	47559	67099	1.37%	0.133%
19	10.019	692	694	697	rVB3	34656	68258	1.39%	0.135%
20	10.088	697	700	702	rBV2	27576	51705	1.05%	0.103%
21	10.213	709	711	713	rVB	172139	174112	3.54%	0.345%
22	10.316	719	720	724	rVB	76214	95437	1.94%	0.189%
23	10.431	727	730	733	rBV	67479	117657	2.39%	0.233%
24	10.568	739	742	744	rBV	2187759	2641054	53.73%	5.236%
25	10.682	750	752	756	rVB2	166074	307129	6.25%	0.609%
26	10.876	766	769	774	rBV5	46071	106542	2.17%	0.211%
27	11.013	777	781	784	rVB3	37489	76072	1.55%	0.151%
28	11.139	787	792	797	rVB3	118360	277253	5.64%	0.550%
29	11.253	800	802	806	rBV2	1582480	2168617	44.12%	4.299%
30	11.333	806	809	811	rVB	111220	135731	2.76%	0.269%
31	11.493	821	823	827	rBV2	40250	74121	1.51%	0.147%
32	11.562	827	829	830	rBV	54357	53201	1.08%	0.105%
33	11.756	844	846	847	rBV	147966	137079	2.79%	0.272%
34	11.791	847	849	851	rVB	129188	175765	3.58%	0.348%

LSC Area Percent Report

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Operator : UM/SJ
Sample : H5463-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5(0-2)

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-BF102616.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.836	851	853	854	rBV2	42289	54753	1.11%	0.109%
36	11.871	854	856	861	rVB2	164720	303377	6.17%	0.601%
37	11.974	861	865	868	rBV2	31617	90786	1.85%	0.180%
38	12.054	870	872	873	rBV	70402	68469	1.39%	0.136%
39	12.236	886	888	892	rVB	46724	71629	1.46%	0.142%
40	12.305	892	894	896	rBV	129244	144514	2.94%	0.287%
41	12.339	896	897	900	rVV2	55238	104106	2.12%	0.206%
42	12.396	900	902	906	rVB2	66755	97667	1.99%	0.194%
43	12.465	906	908	911	rBV	977182	859893	17.49%	1.705%
44	12.614	918	921	925	rBV5	39595	101073	2.06%	0.200%
45	12.694	925	928	930	rVV	722116	831645	16.92%	1.649%
46	12.751	932	933	935	rVB	65608	64975	1.32%	0.129%
47	12.842	938	941	944	rVV	3680655	3564614	72.52%	7.067%
48	12.911	944	947	951	rVV4	92941	198180	4.03%	0.393%
49	13.025	953	957	959	rVV2	122866	271979	5.53%	0.539%
50	13.094	961	963	964	rVV2	51772	76400	1.55%	0.151%
51	13.128	964	966	968	rVV	138176	170351	3.47%	0.338%
52	13.219	972	974	975	rVV	69984	74617	1.52%	0.148%
53	13.254	975	977	979	rVV2	47471	95321	1.94%	0.189%
54	13.322	981	983	986	rVB2	46379	83203	1.69%	0.165%
55	13.528	999	1001	1003	rBV	71639	91216	1.86%	0.181%
56	13.642	1008	1011	1012	rBV	70382	123768	2.52%	0.245%
57	13.745	1018	1020	1024	rVB4	269723	354528	7.21%	0.703%
58	13.894	1030	1033	1039	rBV2	1030137	1799637	36.61%	3.568%
59	13.997	1040	1042	1043	rVB	54311	51504	1.05%	0.102%
60	14.648	1097	1099	1100	rBV	53451	66218	1.35%	0.131%
61	14.740	1105	1107	1110	rVB2	83093	132856	2.70%	0.263%
62	14.900	1118	1121	1126	rBV	272307	587171	11.95%	1.164%
63	15.174	1142	1145	1148	rBV	147453	207958	4.23%	0.412%
64	15.231	1148	1150	1153	rVV	246783	342504	6.97%	0.679%
65	15.288	1153	1155	1162	rVB	787773	1078272	21.94%	2.138%
66	16.614	1268	1271	1277	rVB2	102383	226665	4.61%	0.449%
67	17.014	1303	1306	1311	rVB	69239	144230	2.93%	0.286%

Sum of corrected areas: 50439200

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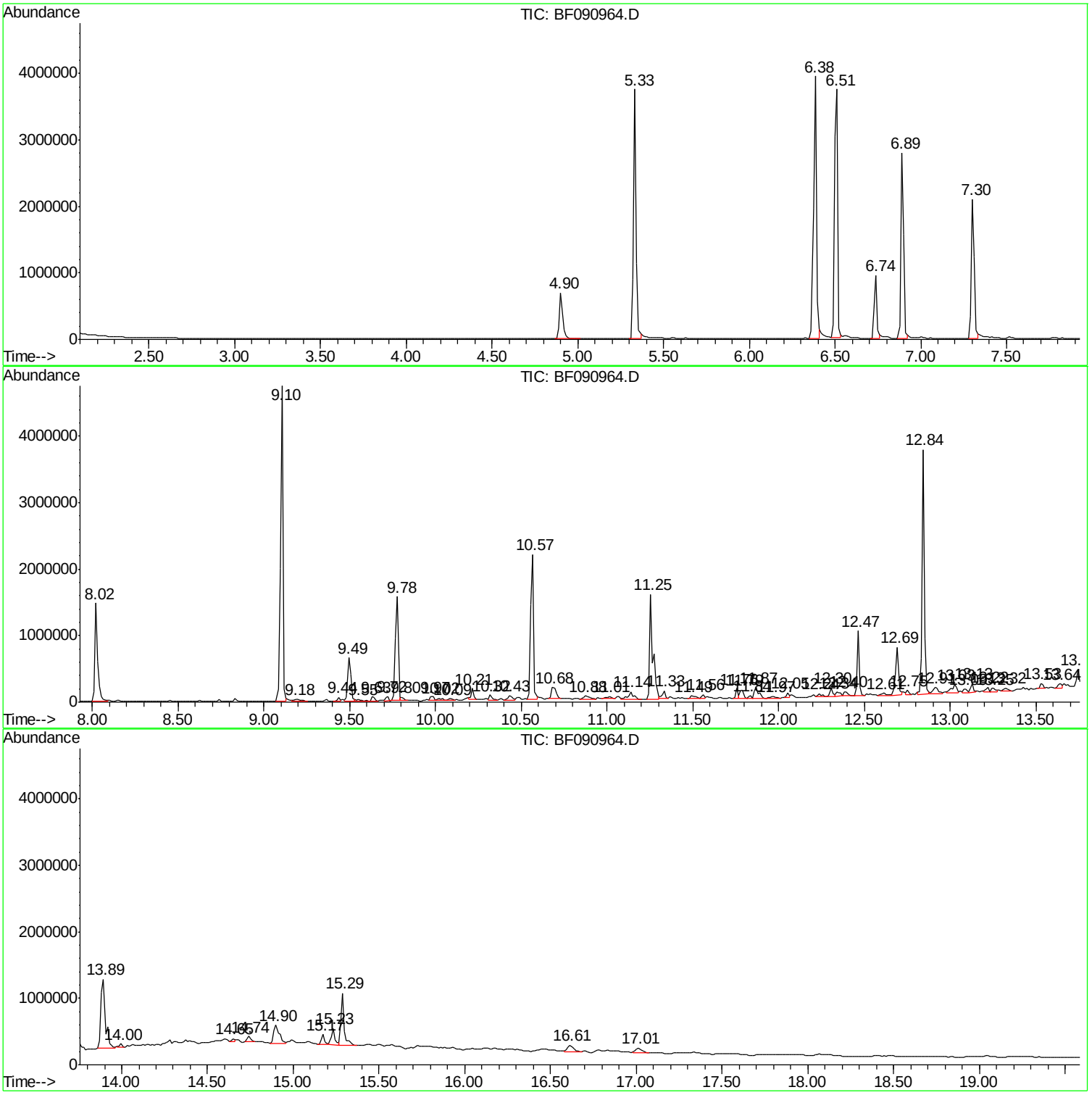
Instrument :
BNA_F
ClientSampleId :
SB-5(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.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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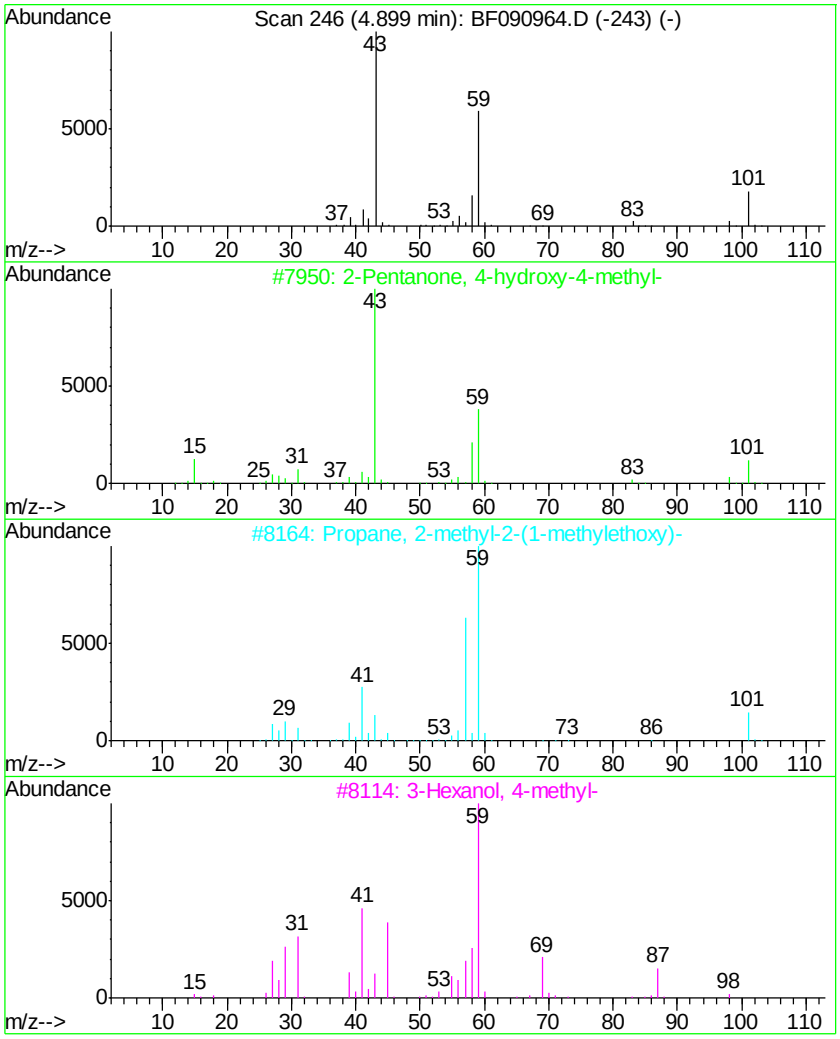
TIC Integration Parameters: LSCINT.P

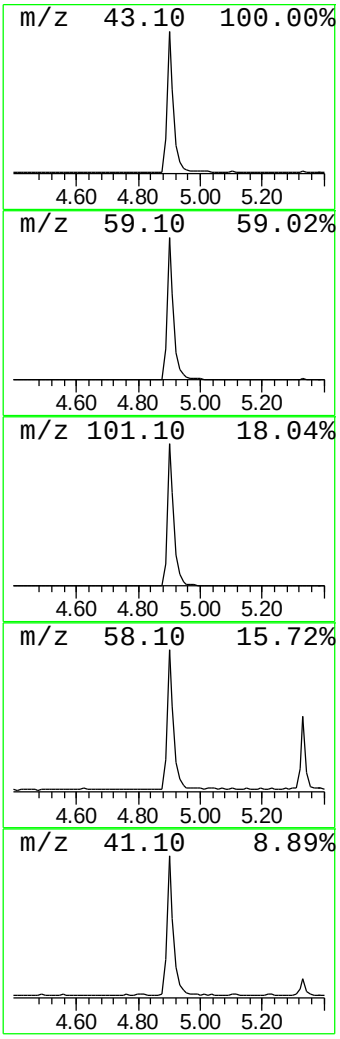
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	19.24 ng	1025600	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110116\
Data File : BF090964.D
Acq On : 1 Nov 2016 21:22
Operator : UM/SJ
Sample : H5463-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

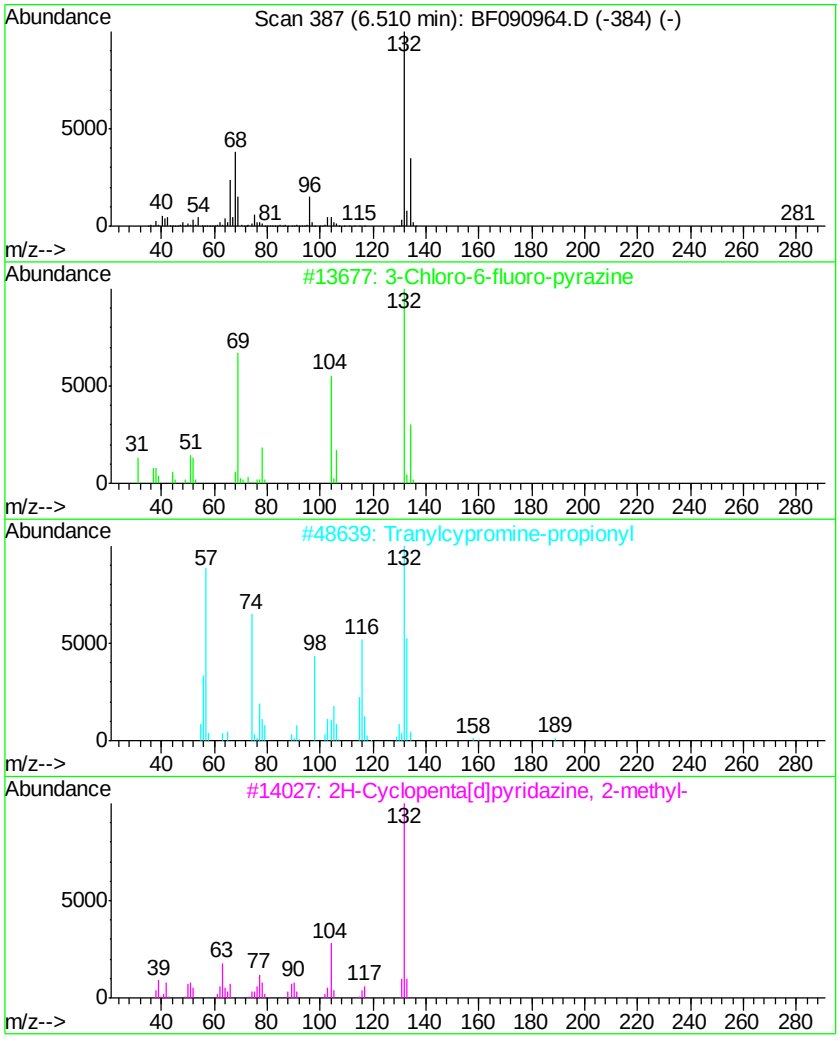
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

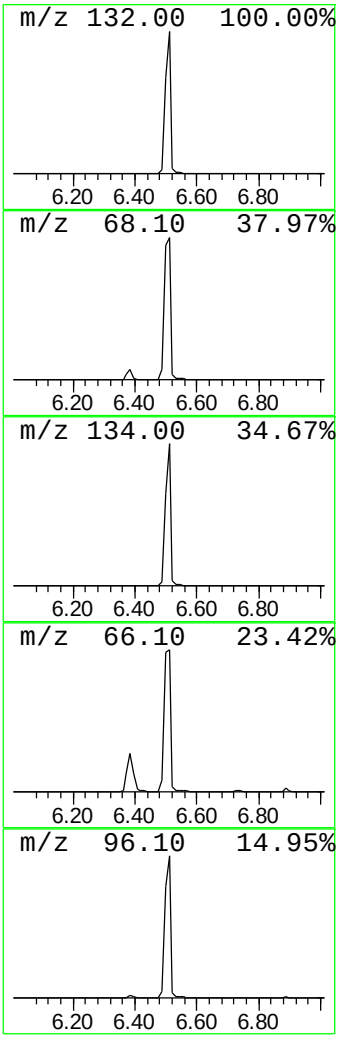
****

Peak Number 2 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	91.58 ng	4880770	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110116\
Data File : BF090964.D
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Operator : UM/SJ
Sample : H5463-10
Misc :
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Instrument : BNA_F
ClientSampleId : SB-5(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.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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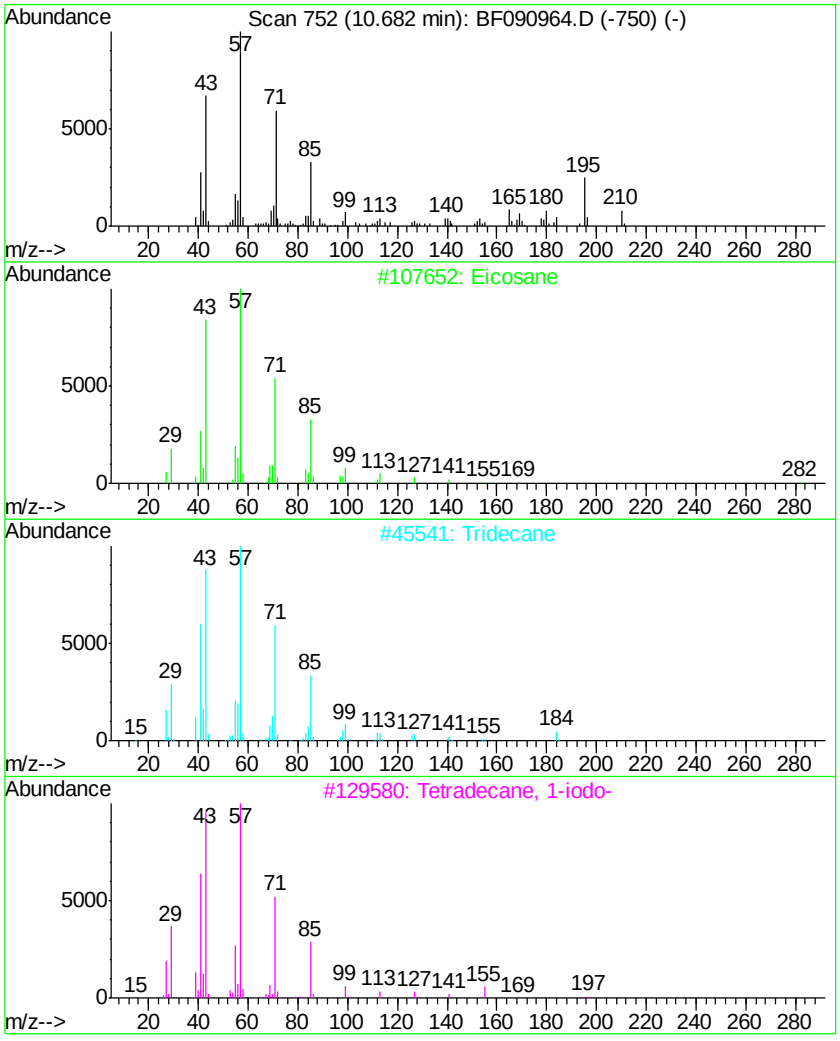
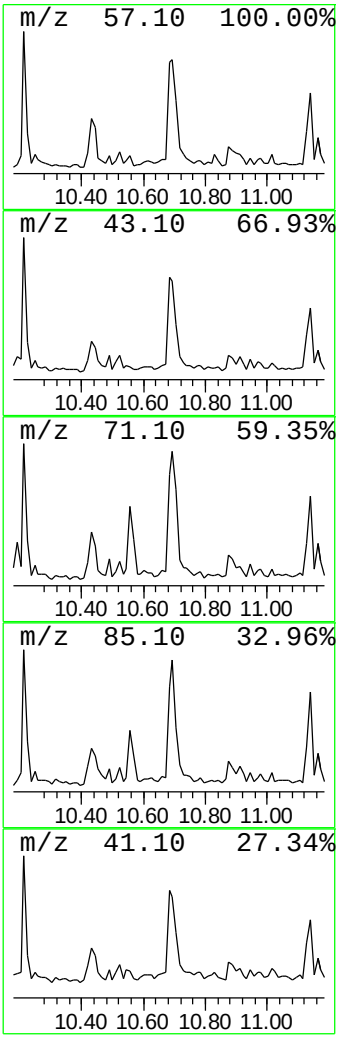
Peak Number 4 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.68	2.83 ng	307129	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	53
2	Tridecane	184	C13H28	000629-50-5	52
3	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	49
4	5-Ethyldecane	170	C12H26	017302-36-2	49
5	Tetradecane	198	C14H30	000629-59-4	49





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110116\
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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
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TIC Library : C:\DATABASE\NIST02.L
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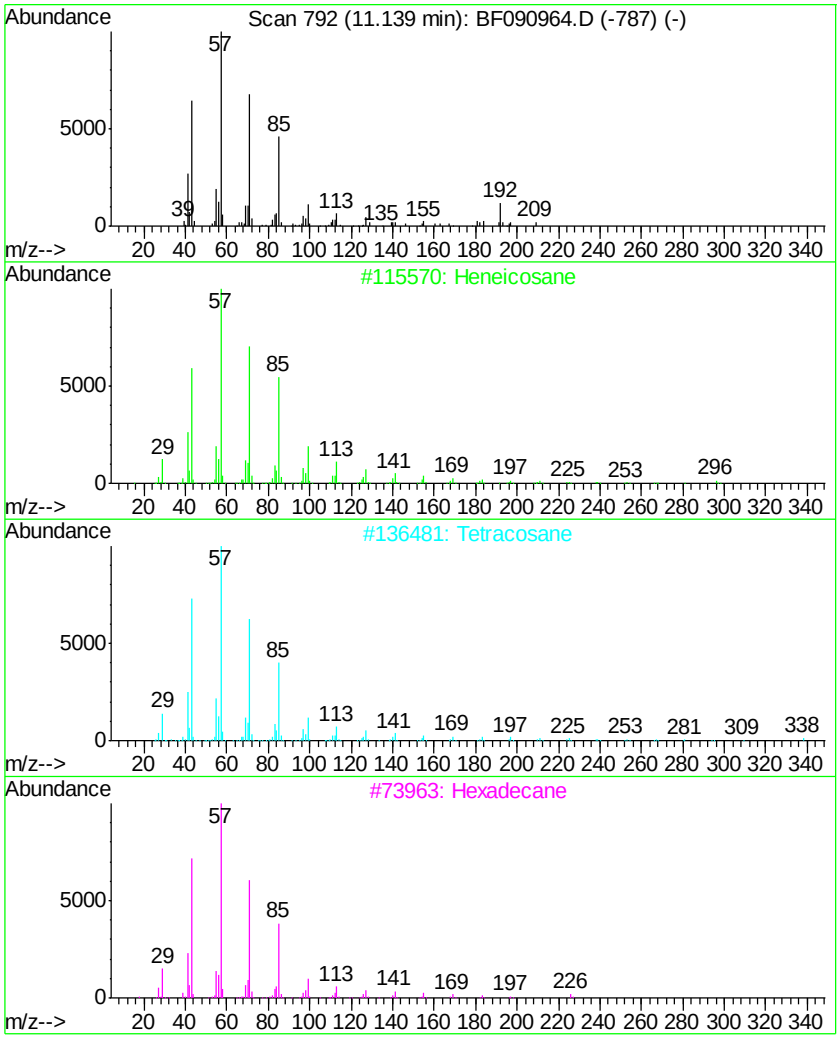
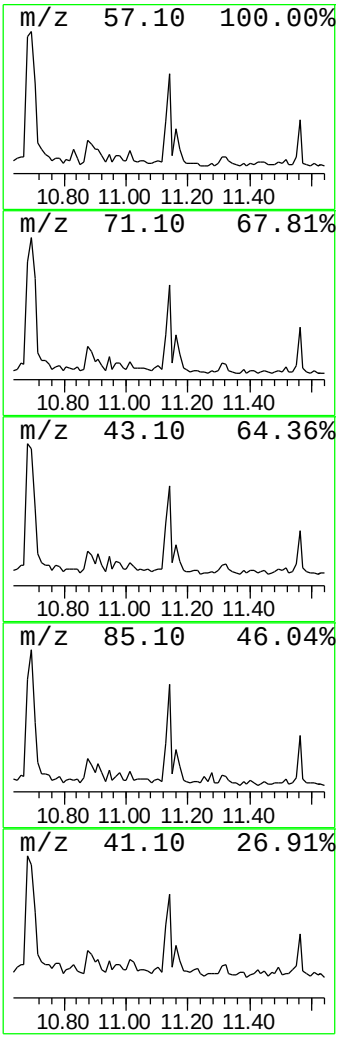
Peak Number 5 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.14	2.56 ng	277253	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	87
2	Tetracosane	338	C24H50	000646-31-1	87
3	Hexadecane	226	C16H34	000544-76-3	86
4	Heptadecane	240	C17H36	000629-78-7	86
5	Pentadecane	212	C15H32	000629-62-9	86





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Sample : H5463-10
Misc :
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Instrument : BNA_F
ClientSampleId : SB-5(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.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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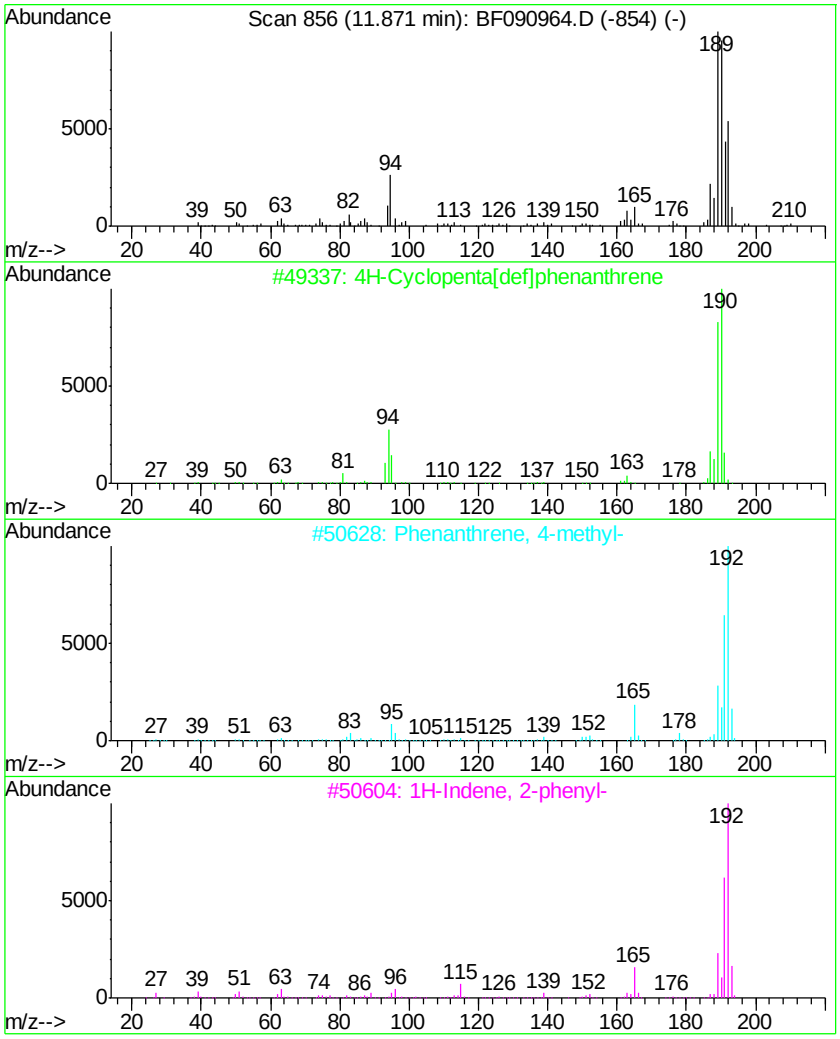
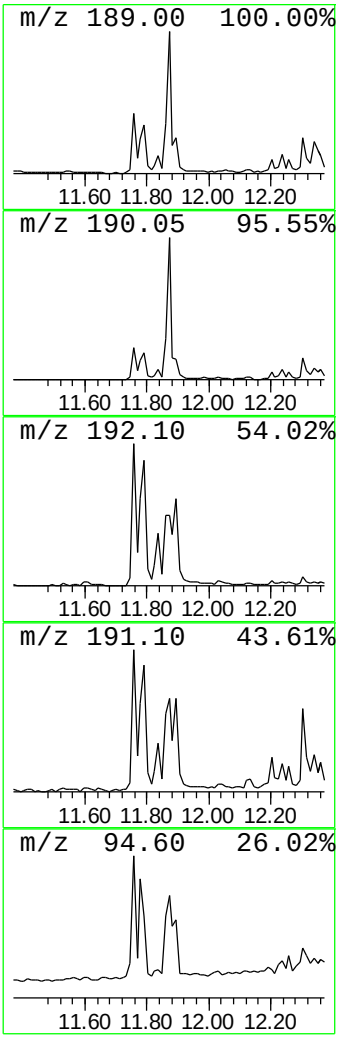
Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	2.80 ng	303377	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	35
3	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	30
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	30
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	25





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Sample : H5463-10
Misc :
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Instrument : BNA_F
ClientSampleId : SB-5(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.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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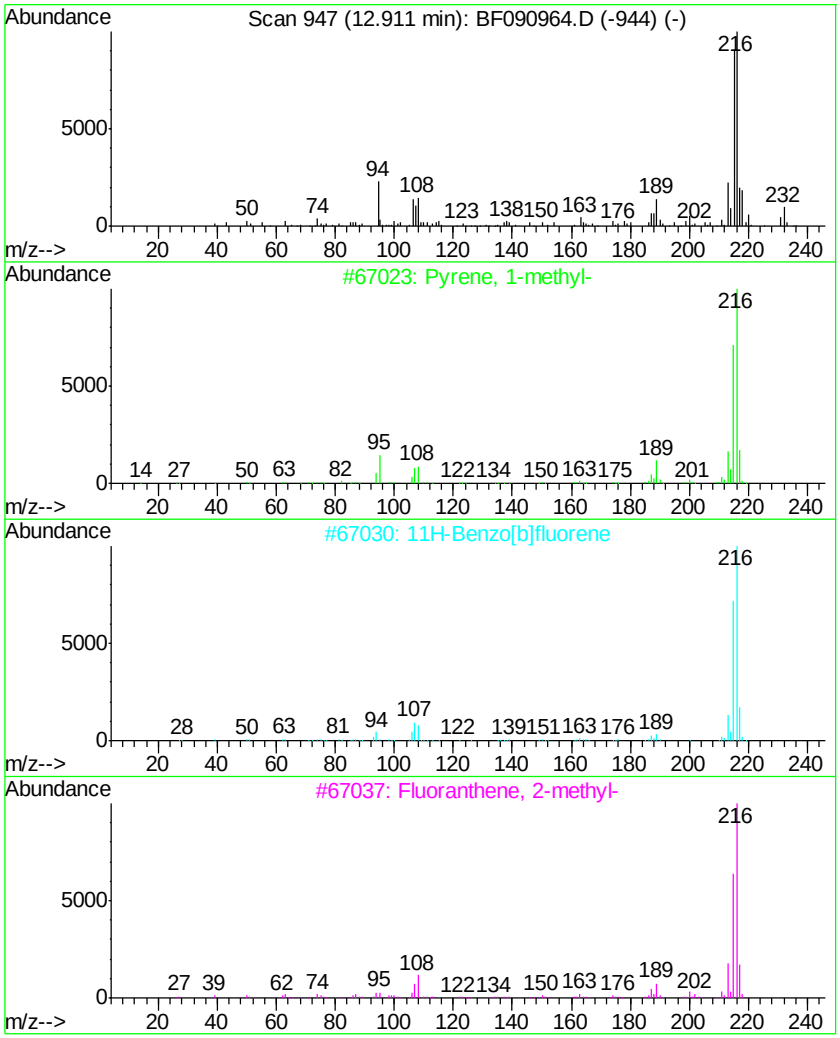
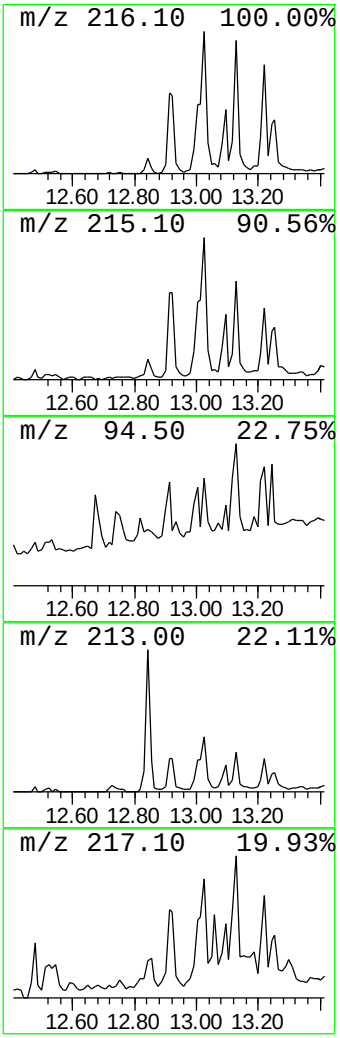
Peak Number 7 Pyrene, 1-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.91	2.20 ng	198180	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	91
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	86
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	76
5	Pyrene, 2-methyl-	216	C17H12	003442-78-2	64





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Sample : H5463-10
Misc :
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Instrument : BNA_F
ClientSampleId : SB-5(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.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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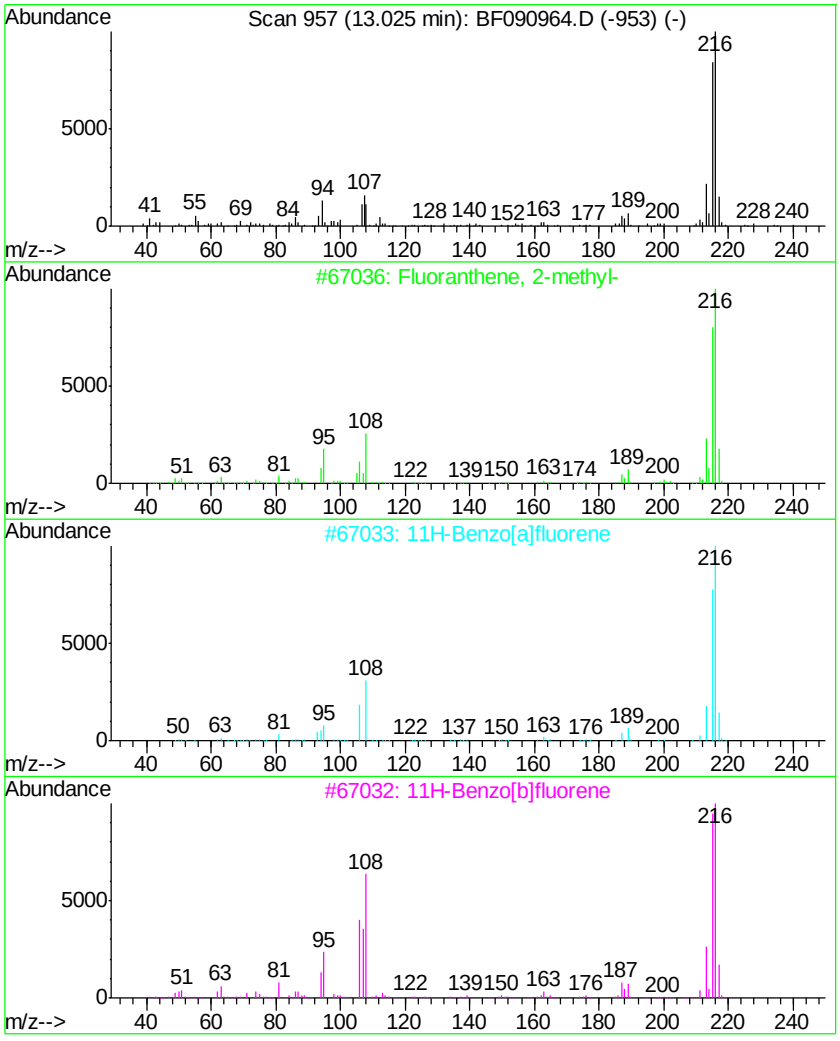
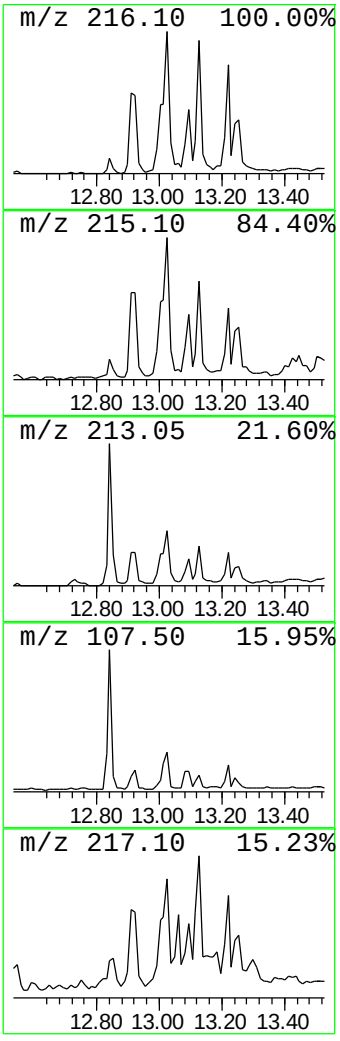
Peak Number 8 Fluoranthene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.03	3.02 ng	271979	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	91
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90
3	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
4	Pyrene, 1-methyl-	216	C17H12	002381-21-7	83
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	81





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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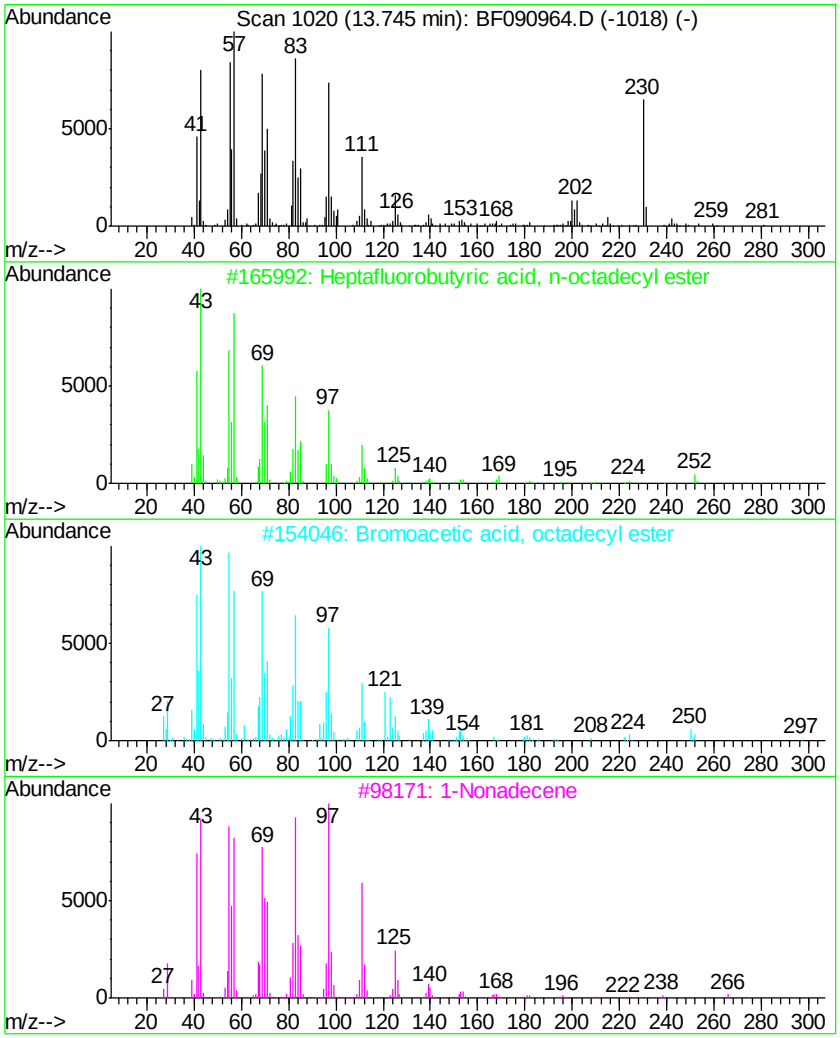
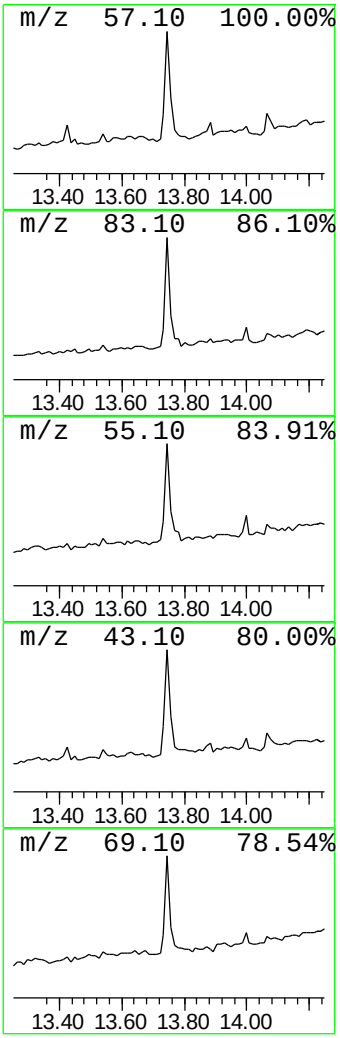
Peak Number 9 Heptafluorobutyric acid, n-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	3.94 ng	354528	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	90
2	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	90
3	1-Nonadecene	266	C19H38	018435-45-5	90
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	90
5	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	90





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110116\
Data File : BF090964.D
Acq On : 1 Nov 2016 21:22
Operator : UM/SJ
Sample : H5463-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.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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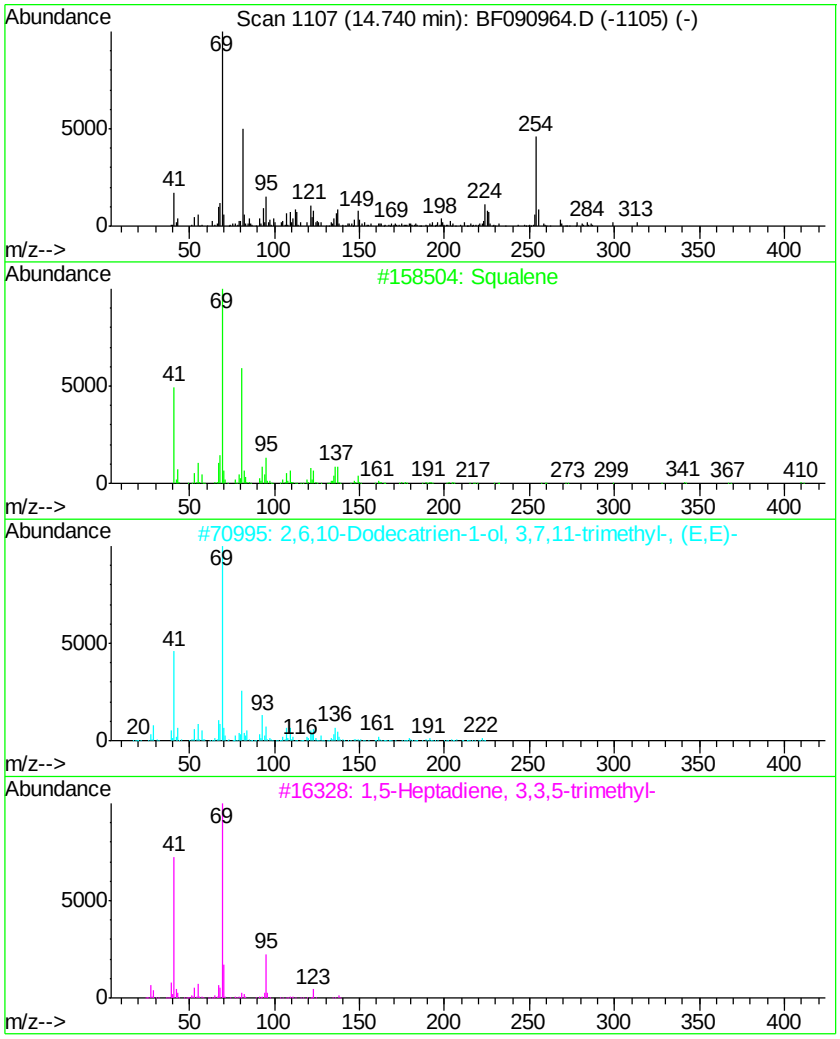
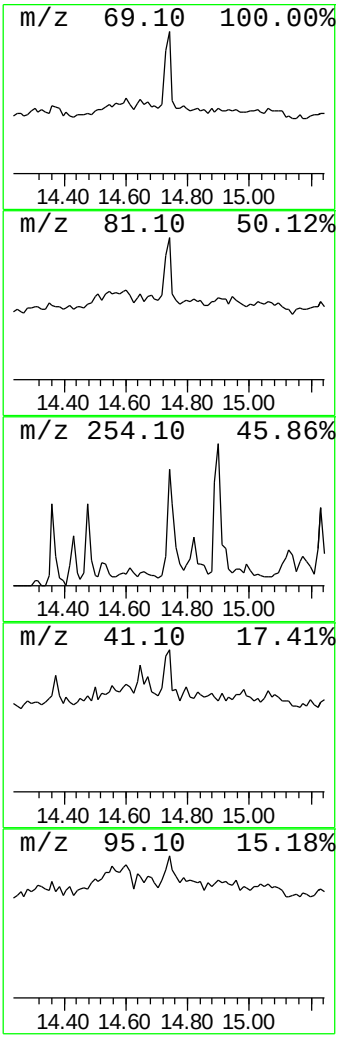
Peak Number 10 Squalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.74	2.46 ng	132856	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	53
2	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	000106-28-5	53
3	1,5-Heptadiene, 3,3,5-trimethyl-	138	C10H18	074630-29-8	43
4	1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	43
5	1,5-Heptadiene, 2,3,6-trimethyl-	138	C10H18	033501-88-1	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110116\
Data File : BF090964.D
Acq On : 1 Nov 2016 21:22
Operator : UM/SJ
Sample : H5463-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.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...	4.90	19.2	ng	1025600	1	6.74	1065880	20.0
unknown6.51	6.51	91.6	ng	4880770	1	6.74	1065880	20.0
Eicosane	10.68	2.8	ng	307129	4	11.25	2168620	20.0
Heneicosane	11.14	2.6	ng	277253	4	11.25	2168620	20.0
4H-Cyclopenta[def...	11.87	2.8	ng	303377	4	11.25	2168620	20.0
Pyrene, 1-methyl-	12.91	2.2	ng	198180	5	13.89	1799640	20.0
Fluoranthene, 2-m...	13.03	3.0	ng	271979	5	13.89	1799640	20.0
Heptafluorobutyri...	13.75	3.9	ng	354528	5	13.89	1799640	20.0
Squalene	14.74	2.5	ng	132856	6	15.29	1078270	20.0