LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070516\
Data File : BF088728.D
Acq On : 6 Jul 2016 3:32
Operator : UM/SJ
Sample : H3881-15
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q6-B8-0-5-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	1.713	9	11	20	rVB	86042	142747	6.37%	0.603%
2	1.838	20	22	35	rVB	575265	1198518	53.51%	5.060%
3	4.947	291	294	299	rBB	88242	131246	5.86%	0.554%
4	5.370	328	331	333	rBV	2015220	2038298	91.00%	8.606%
5	6.410	419	422	425	rVB	1808154	1918635	85.66%	8.100%
6	6.547	431	434	436	rBV	1602697	2190903	97.82%	9.250%
7	6.776	452	454	456	rBV	712758	613223	27.38%	2.589%
8	6.936	465	468	470	rBB	1489774	1721742	76.87%	7.269%
9	7.336	500	503	506	rBV	1184287	1230105	54.92%	5.193%
10	8.056	564	566	569	rBV	853242	754775	33.70%	3.187%
11	9.131	658	660	663	rBV	1590787	2239839	100.00%	9.457%
12	9.531	693	695	697	rBV	376799	328697	14.68%	1.388%
13	9.748	713	714	717	rBV	25801	24672	1.10%	0.104%
14	9.805	717	719	721	rBV	874597	771443	34.44%	3.257%
15	10.251	756	758	760	rVB	47820	36101	1.61%	0.152%
16	10.594	785	788	790	rBV	1180848	1158847	51.74%	4.893%
17	10.719	797	799	803	rVB	59673	61973	2.77%	0.262%
18	11.165	837	838	844	rVB	72073	84396	3.77%	0.356%
19	11.279	846	848	852	rVV	604138	853156	38.09%	3.602%
20	11.359	852	855	856	rVV2	53309	59915	2.67%	0.253%
21	11.508	866	868	870	rVV	22419	22514	1.01%	0.095%
22	11.588	873	875	879	rVB2	32861	45077	2.01%	0.190%
23	11.782	890	892	893	rBV	35265	28634	1.28%	0.121%
24	11.805	893	894	897	rVB	32589	38907	1.74%	0.164%
25	11.897	900	902	906	rVB	45769	74250	3.31%	0.313%
26	11.999	906	911	915	rBV4	10373	28916	1.29%	0.122%
27	12.079	916	918	922	rVB2	25440	46168	2.06%	0.195%
28	12.331	938	940	942	rBV	22651	26646	1.19%	0.112%
29	12.491	951	954	956	rBV	400259	391946	17.50%	1.655%
30	12.708	971	973	976	rVV	249097	409466	18.28%	1.729%
31	12.777	976	979	981	rVB3	26155	43928	1.96%	0.185%
32	12.834	982	984	985	rBV	22324	23643	1.06%	0.100%
33	12.868	985	987	989	rVB	1746674	1577776	70.44%	6.661%
34	12.937	989	993	994	rBV2	23178	29963	1.34%	0.127%

LSC Area Percent Report

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Data File : BF088728.D
Acq On : 6 Jul 2016 3:32
Operator : UM/SJ
Sample : H3881-15
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q6-B8-0-5-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	13.040	997	1002	1004	rBV2	49591	86264	3.85%	0.364%
36	13.108	1006	1008	1010	rBV	49435	47880	2.14%	0.202%
37	13.142	1010	1011	1015	rVB2	38473	45322	2.02%	0.191%
38	13.405	1032	1034	1036	rBV	35273	36206	1.62%	0.153%
39	13.451	1036	1038	1043	rVB3	21784	35818	1.60%	0.151%
40	13.542	1043	1046	1051	rBV	43128	70177	3.13%	0.296%
41	13.657	1054	1056	1057	rBV2	39579	52227	2.33%	0.221%
42	13.691	1057	1059	1063	rVB2	14079	29671	1.32%	0.125%
43	13.748	1063	1064	1066	rBV	33258	28026	1.25%	0.118%
44	13.782	1066	1067	1074	rVB4	58212	98282	4.39%	0.415%
45	13.908	1074	1078	1079	rBV2	718223	858397	38.32%	3.624%
46	14.011	1085	1087	1089	rBV	30292	32444	1.45%	0.137%
47	14.091	1093	1094	1095	rVV	34456	28583	1.28%	0.121%
48	14.125	1095	1097	1099	rVB2	21679	31835	1.42%	0.134%
49	14.285	1107	1111	1113	rBV	30670	67924	3.03%	0.287%
50	14.331	1113	1115	1116	rVB2	26304	31744	1.42%	0.134%
51	14.411	1118	1122	1123	rBV2	22762	67172	3.00%	0.284%
52	14.754	1150	1152	1156	rVB3	29998	48250	2.15%	0.204%
53	14.823	1156	1158	1160	rBV2	31837	32035	1.43%	0.135%
54	14.903	1163	1165	1170	rBV	160963	352253	15.73%	1.487%
55	15.005	1171	1174	1176	rVB	59925	75075	3.35%	0.317%
56	15.177	1187	1189	1192	rVB	84839	124757	5.57%	0.527%
57	15.234	1192	1194	1197	rBV	106743	143188	6.39%	0.605%
58	15.303	1197	1200	1202	rBV	383915	528081	23.58%	2.230%
59	15.748	1236	1239	1243	rBV2	33688	57506	2.57%	0.243%
60	16.468	1299	1302	1310	rVV3	25003	70053	3.13%	0.296%
61	16.617	1313	1315	1319	rVB2	54269	103756	4.63%	0.438%
62	17.017	1347	1350	1358	rVB	39499	92342	4.12%	0.390%
63	18.526	1478	1482	1488	rVB3	19720	63216	2.82%	0.267%

Sum of corrected areas: 23685549

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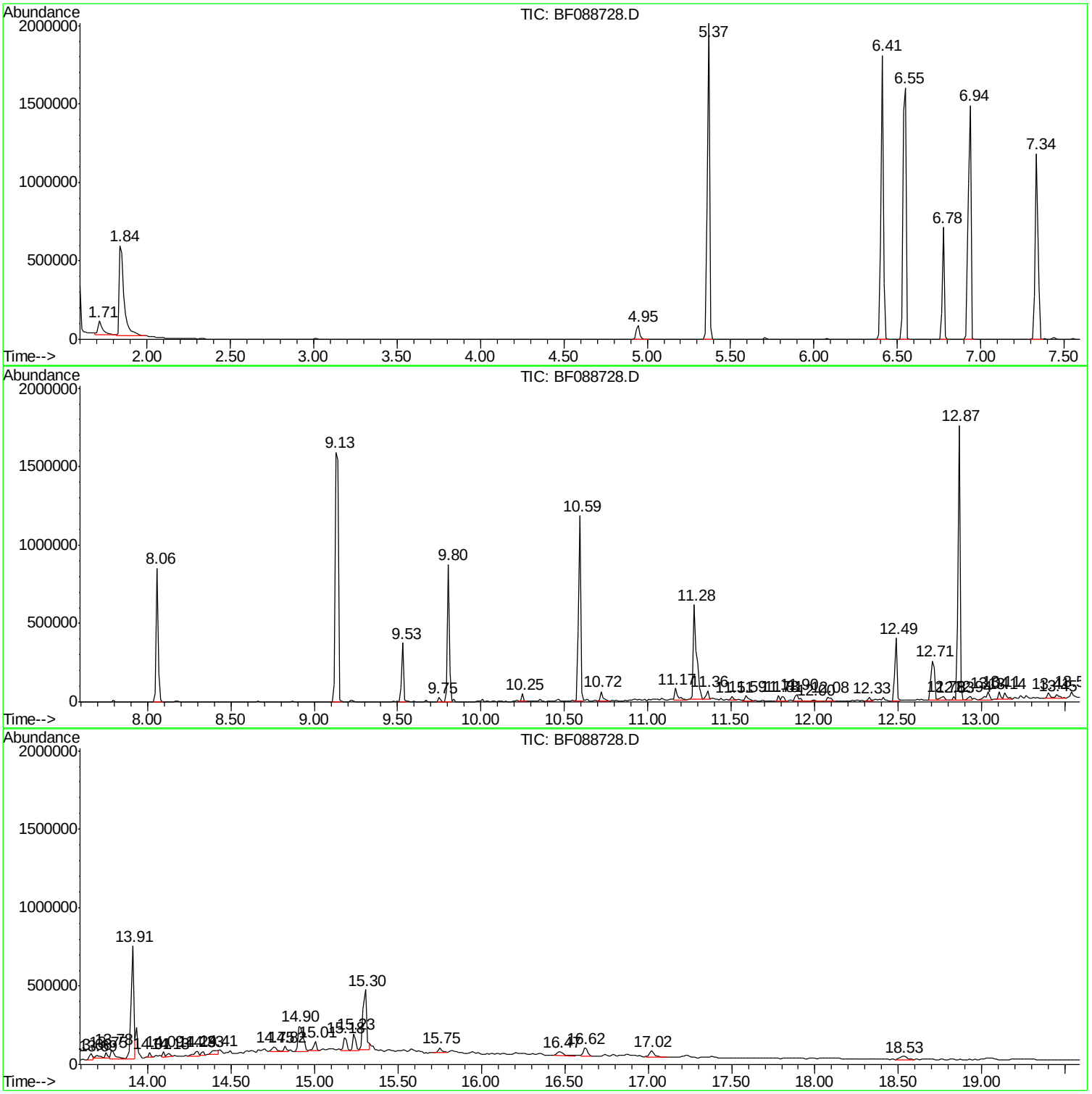
Instrument :
BNA_F
ClientSampleId :
Q6-B8-0-5-C

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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Instrument : BNA_F
ClientSampleId : Q6-B8-0-5-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
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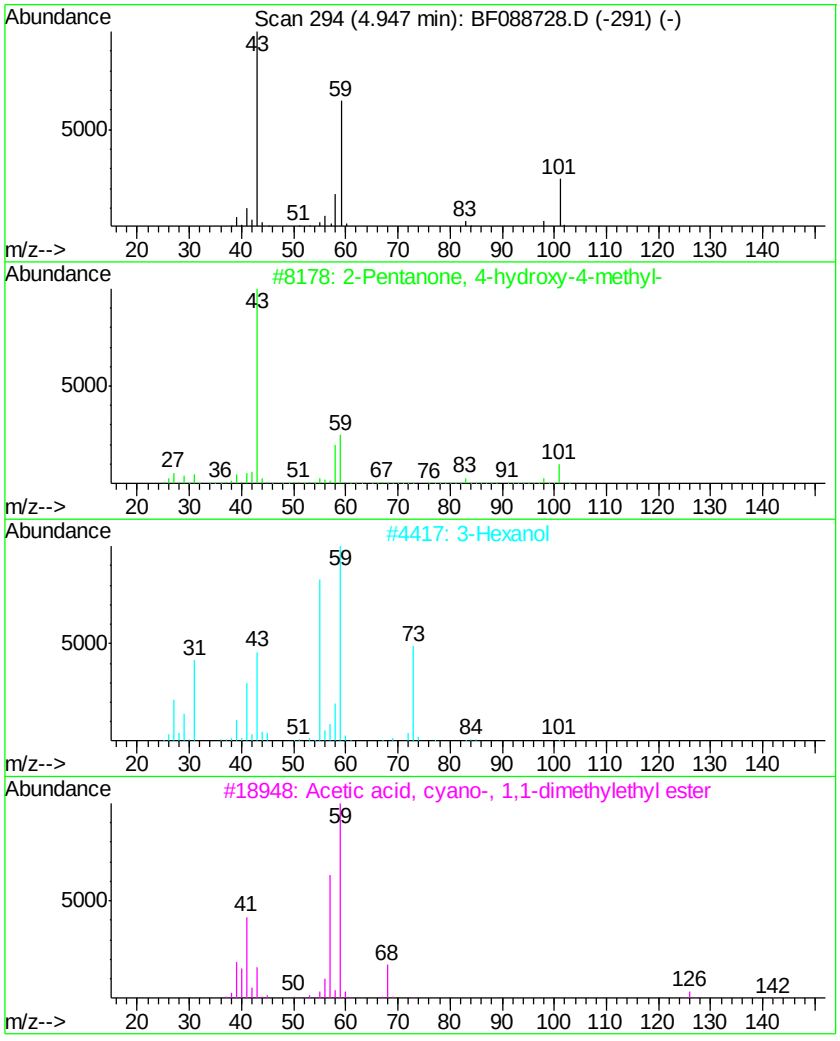
TIC Integration Parameters: LSCINT.P

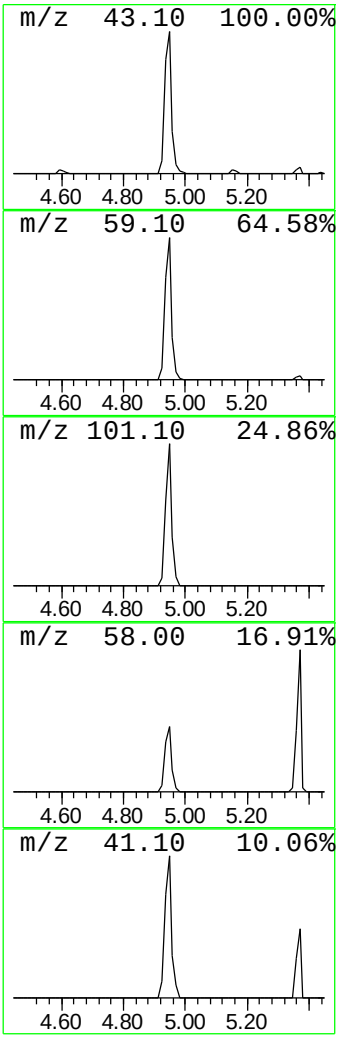
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.95	4.28 ng	131246	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Hexanol	102	C6H14O	000623-37-0	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070516\
Data File : BF088728.D
Acq On : 6 Jul 2016 3:32
Operator : UM/SJ
Sample : H3881-15
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q6-B8-0-5-C

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

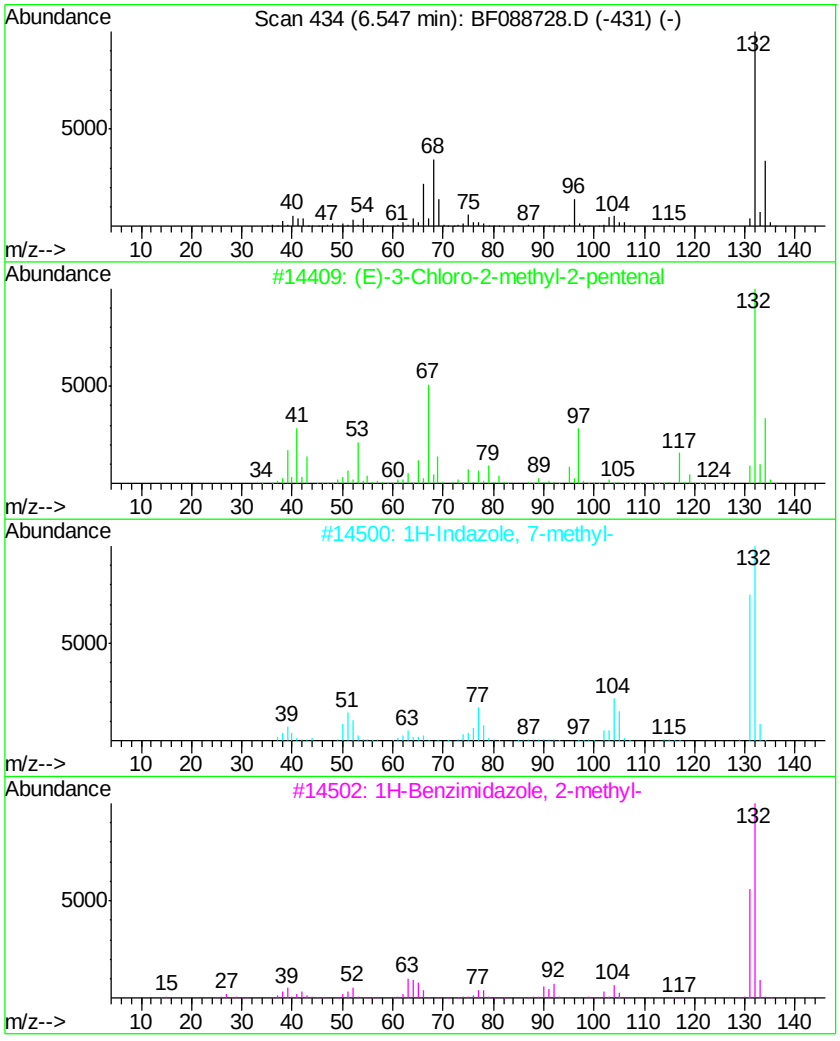
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

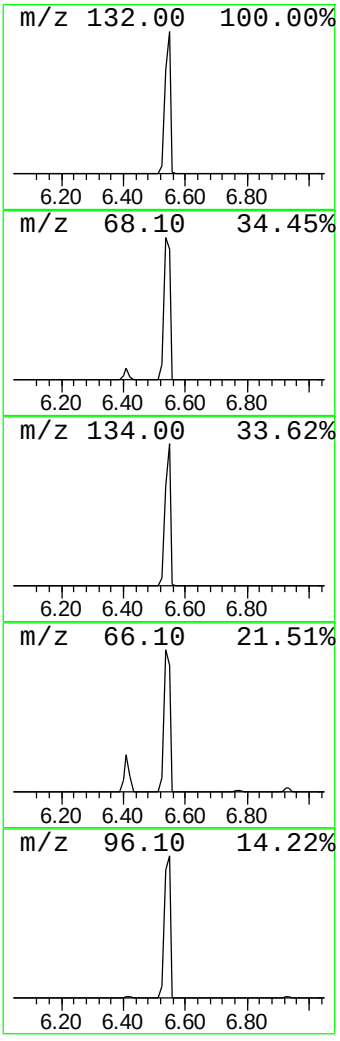
****

Peak Number 4 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	71.46 ng	2190900	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
2	1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	12
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
4	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Operator : UM/SJ
Sample : H3881-15
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q6-B8-0-5-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
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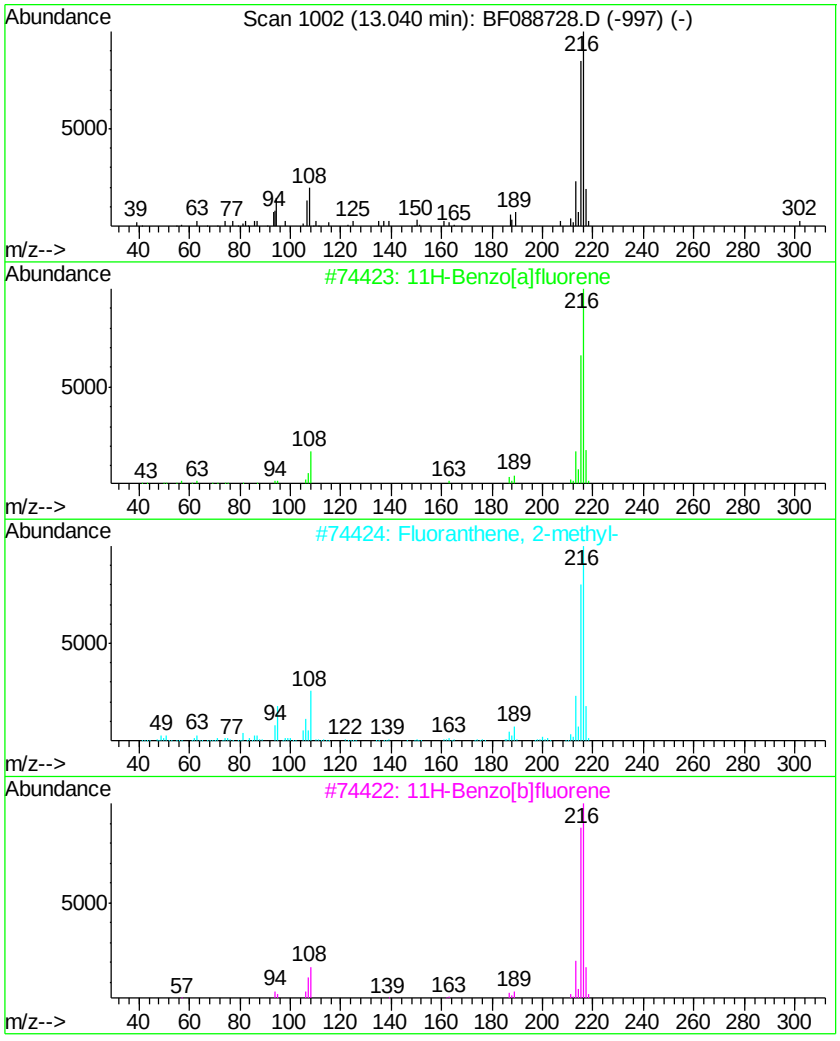
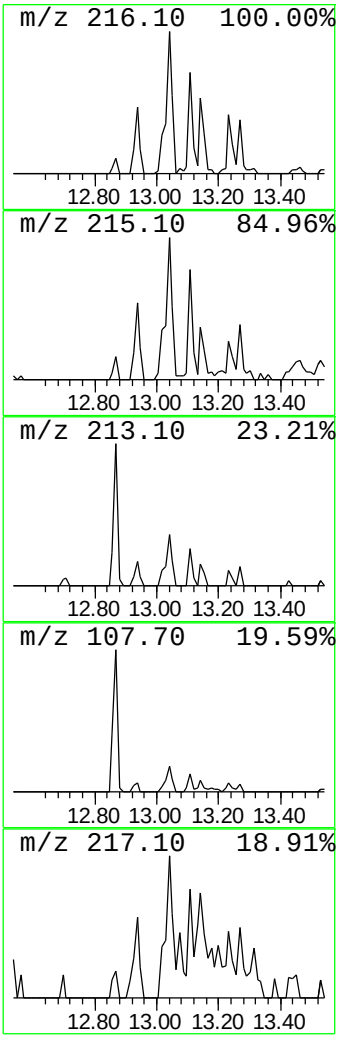
Peak Number 6 11H-Benzo[a]fluorene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.04	2.01 ng	86264	Chrysene-d12	13.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	94
2	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	93
3	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	93
4	Pyrene, 1-methyl-	216	C17H12	002381-21-7	91
5	Pyrene, 2-methyl-	216	C17H12	003442-78-2	87





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Acq On : 6 Jul 2016 3:32
Operator : UM/SJ
Sample : H3881-15
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q6-B8-0-5-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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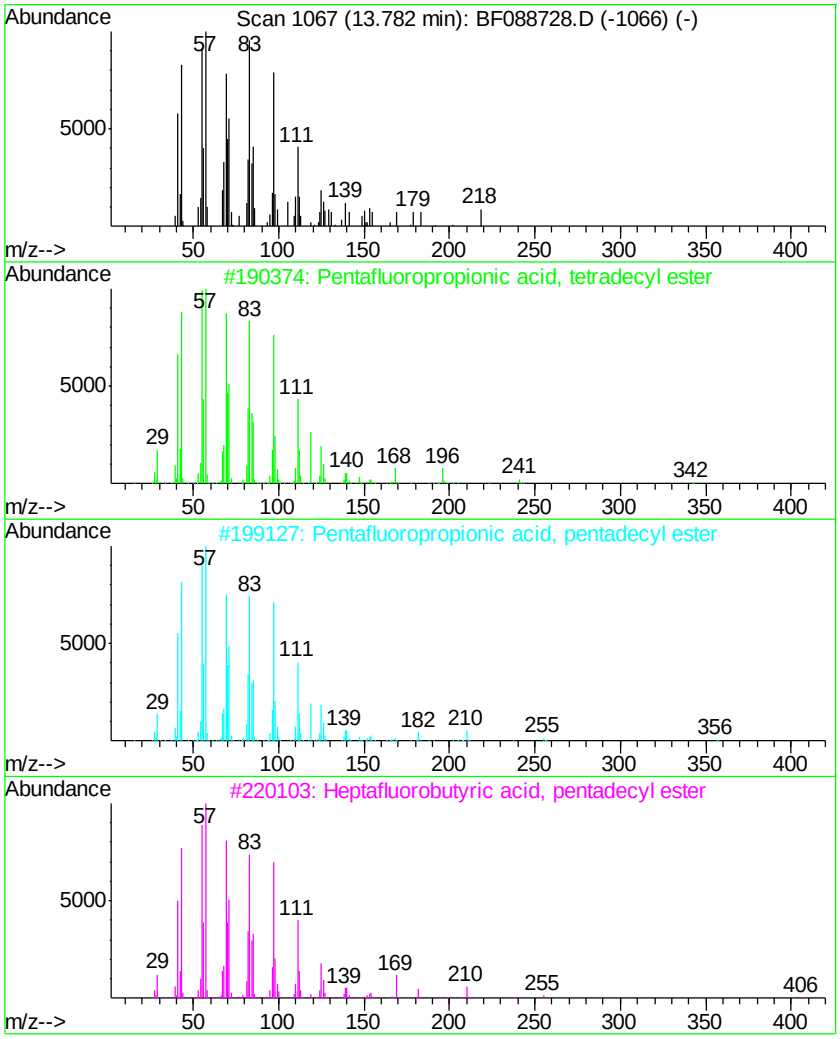
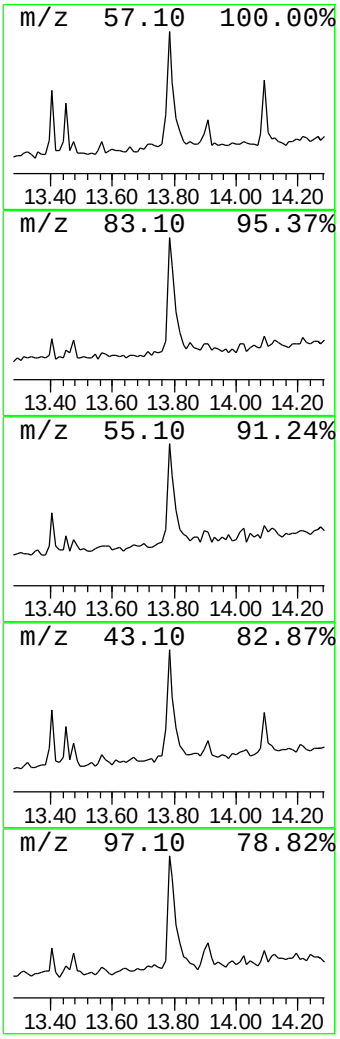
Peak Number 7 Pentafluoropropionic acid, ... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.78	2.29 ng	98282	Chrysene-d12	13.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	94
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	90





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Instrument : BNA_F
ClientSampleId : Q6-B8-0-5-C

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

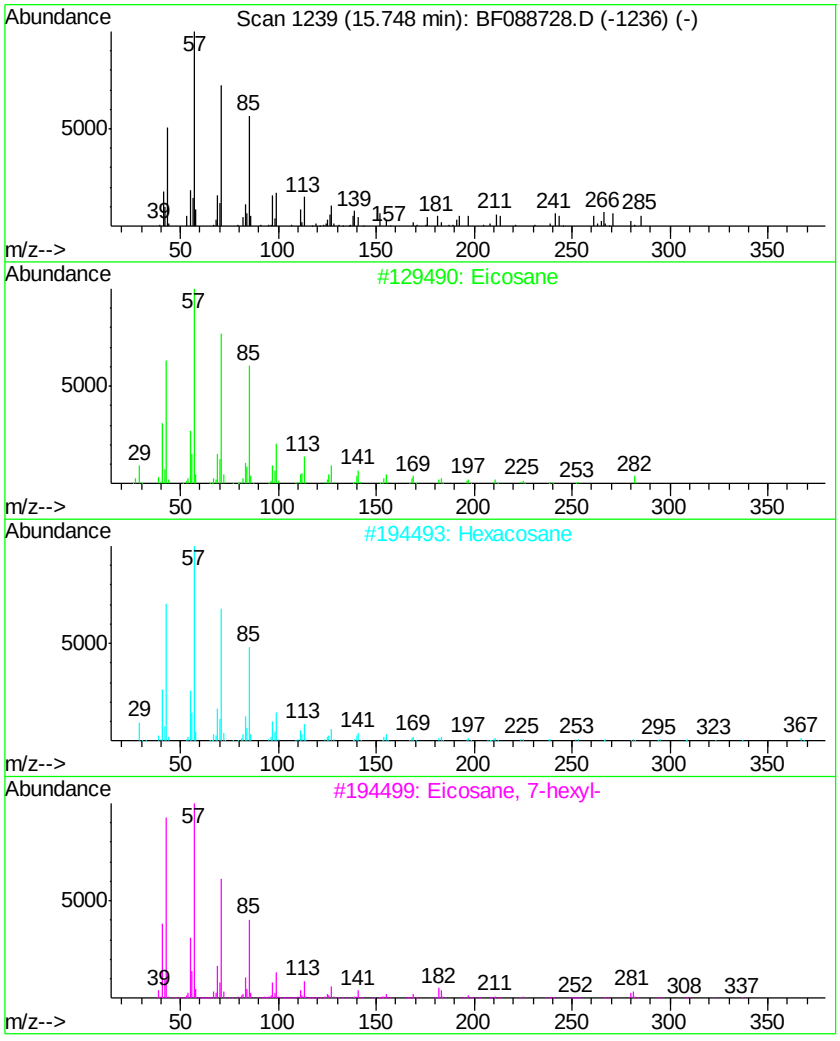
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

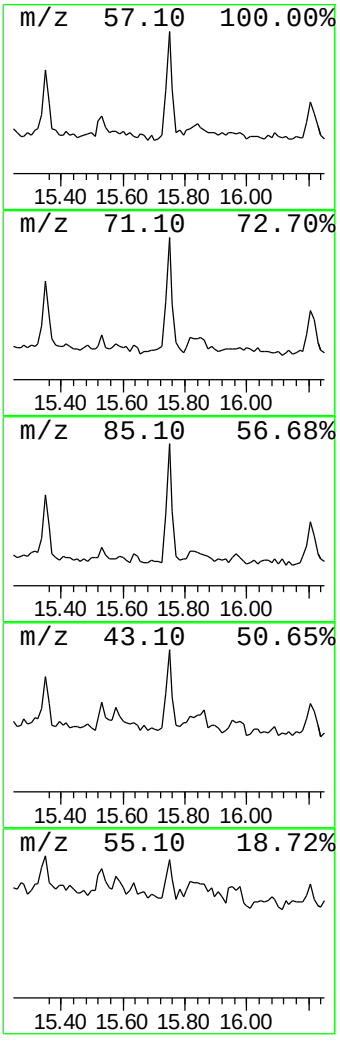
****

Peak Number 10 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.75	2.18 ng	57506	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexacosane	366	C26H54	000630-01-3	90
3	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	87
4	Pentacosane	352	C25H52	000629-99-2	86
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86





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Misc :
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Instrument : BNA_F
ClientSampleId : Q6-B8-0-5-C

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

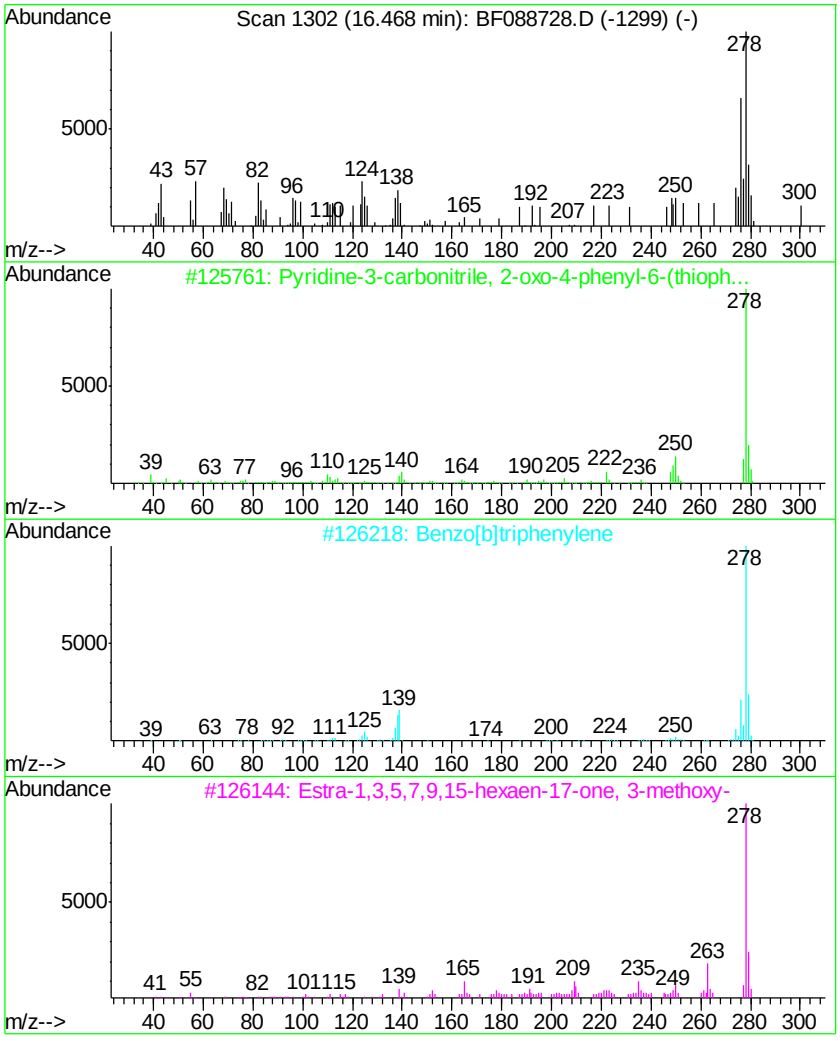
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

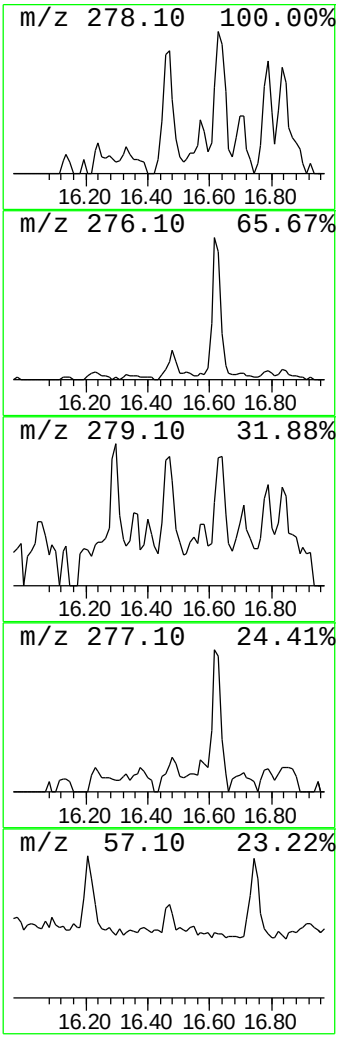
****

Peak Number 11 unknown16.47 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.47	2.65 ng	70053	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine-3-carbonitrile, 2-oxo-4...	278	C16H10N2OS	1000304-72-3	46
2	Benzo[b]triphenylene	278	C22H14	000215-58-7	41
3	Estra-1,3,5,7,9,15-hexaen-17-one...	278	C19H18O2	056588-53-5	38
4	Pentaphene	278	C22H14	000222-93-5	38
5	Dibenz[a,h]anthracene	278	C22H14	000053-70-3	35





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Instrument : BNA_F
ClientSampleId : Q6-B8-0-5-C

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

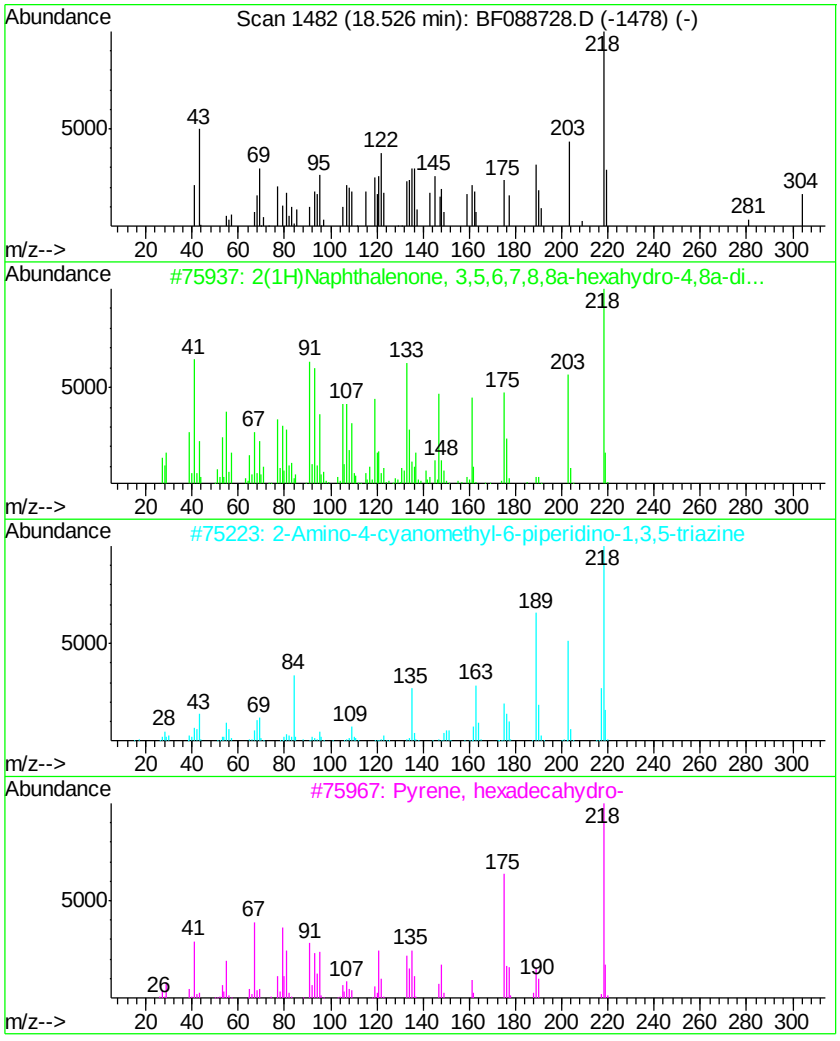
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

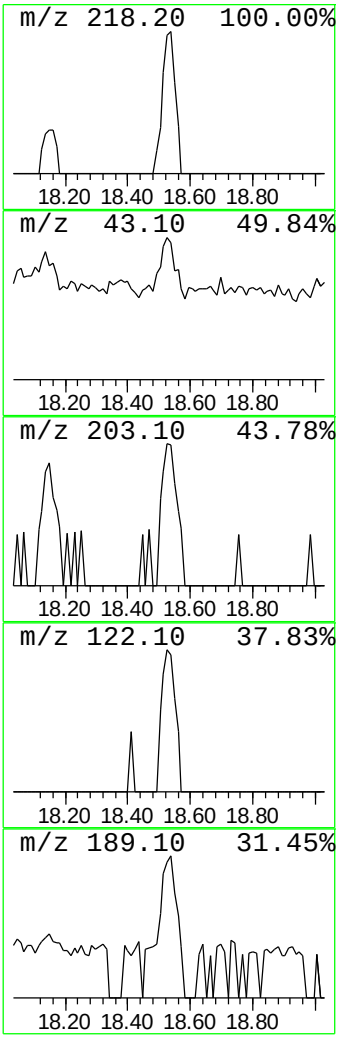
****

Peak Number 12 2(1H)Naphthalenone, 3,5,6,7... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.53	2.39 ng	63216	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)Naphthalenone, 3,5,6,7,8,8a...	218	C15H22O	1000188-66-5	64
2	2-Amino-4-cyanomethyl-6-piperidi...	218	C10H14N6	1000241-05-9	52
3	Pyrene, hexadecahydro-	218	C16H26	002435-85-0	45
4	Acetic acid, 3-hydroxy-7-isoprop...	278	C17H26O3	1000187-37-6	45
5	5(1H)-Azulenone, 2,4,6,7,8,8a-he...	218	C15H22O	006754-66-1	43





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_F
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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...	4.95	4.3	ng	131246	1	6.78	613223	20.0
unknown6.55	6.55	71.5	ng	2190900	1	6.78	613223	20.0
11H-Benzo[a]fluorene	13.04	2.0	ng	86264	5	13.91	858397	20.0
Pentafluoropropio...	13.78	2.3	ng	98282	5	13.91	858397	20.0
Eicosane	15.75	2.2	ng	57506	6	15.30	528081	20.0
unknown16.47	16.47	2.6	ng	70053	6	15.30	528081	20.0
2(1H)Naphthalenon...	18.53	2.4	ng	63216	6	15.30	528081	20.0