LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\Data\BF031617\
Data File : BF093718.D
Acq On : 16 Mar 2017 20:46
Operator : SJ/MA
Sample : I2266-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP6

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-BF030717.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	4.847	256	259	271	rBV	232367	504857	10.41%	0.929%
2	5.293	296	298	325	rBV	2628133	4698255	96.86%	8.644%
3	6.356	389	391	399	rBV	3523999	4850733	100.00%	8.924%
4	6.470	399	401	404	rVB	3836596	4479495	92.35%	8.241%
5	6.687	419	420	428	rBV	787792	1196338	24.66%	2.201%
6	6.847	432	434	449	rVB	3308359	3249090	66.98%	5.978%
7	7.270	469	471	484	rBV	2707537	3012142	62.10%	5.542%
8	7.990	531	534	544	rBV	1205960	1621265	33.42%	2.983%
9	9.065	625	628	630	rBV	4373705	4478539	92.33%	8.240%
10	9.408	655	658	661	rBV2	25684	51003	1.05%	0.094%
11	9.465	661	663	667	rVB	760411	665312	13.72%	1.224%
12	9.602	674	675	679	rBV	55536	56297	1.16%	0.104%
13	9.739	684	687	689	rVV	1543059	1787320	36.85%	3.288%
14	9.773	689	690	692	rVB	104559	79191	1.63%	0.146%
15	10.162	720	724	726	rBV2	111520	143521	2.96%	0.264%
16	10.288	732	735	738	rBV2	74346	104946	2.16%	0.193%
17	10.379	738	743	746	rBV3	42235	94058	1.94%	0.173%
18	10.528	754	756	759	rBV	2190259	2387965	49.23%	4.393%
19	10.642	764	766	769	rBV2	132752	212575	4.38%	0.391%
20	10.836	780	783	784	rBV2	39641	61034	1.26%	0.112%
21	10.962	792	794	799	rBV4	39339	75946	1.57%	0.140%
22	11.054	799	802	803	rVV	46965	65362	1.35%	0.120%
23	11.076	803	804	806	rVV	121382	164926	3.40%	0.303%
24	11.122	806	808	810	rVB2	65377	90885	1.87%	0.167%
25	11.225	815	817	821	rBV2	1367023	2787926	57.47%	5.129%
26	11.305	821	824	827	rVB	178477	239750	4.94%	0.441%
27	11.476	836	839	840	rBV2	101626	143131	2.95%	0.263%
28	11.511	840	842	843	rVB	125350	128436	2.65%	0.236%
29	11.728	859	861	862	rBV	98804	128661	2.65%	0.237%
30	11.751	862	863	866	rVV	222349	286799	5.91%	0.528%
31	11.808	866	868	869	rVV	58077	94010	1.94%	0.173%
32	11.831	869	870	875	rVV	216383	328994	6.78%	0.605%
33	12.014	885	886	889	rVB	99116	100183	2.07%	0.184%
34	12.071	889	891	895	rVB2	79569	114234	2.35%	0.210%

LSC Area Percent Report

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Sample : I2266-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP6

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-BF030717.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.162	895	899	901	rBV3	41875	80129	1.65%	0.147%
36	12.277	907	909	910	rBV	79764	107177	2.21%	0.197%
37	12.311	910	912	915	rVV2	50802	99767	2.06%	0.184%
38	12.379	915	918	920	rVB2	71510	123043	2.54%	0.226%
39	12.437	920	923	925	rBV	1292724	1535848	31.66%	2.826%
40	12.585	934	936	939	rBV2	78313	110914	2.29%	0.204%
41	12.654	939	942	945	rVV2	963081	1569190	32.35%	2.887%
42	12.722	945	948	950	rVB2	66192	105290	2.17%	0.194%
43	12.802	952	955	957	rBV	3547836	3611779	74.46%	6.645%
44	12.848	957	959	960	rVB	38110	51743	1.07%	0.095%
45	12.882	960	962	964	rVB2	76341	136427	2.81%	0.251%
46	12.997	968	972	973	rBV2	87860	193142	3.98%	0.355%
47	13.099	979	981	984	rVV3	121280	176104	3.63%	0.324%
48	13.191	987	989	990	rBV	65740	62517	1.29%	0.115%
49	13.225	990	992	996	rVB2	62924	98287	2.03%	0.181%
50	13.362	1002	1004	1006	rBV2	48744	61446	1.27%	0.113%
51	13.522	1015	1018	1020	rBV	79916	129187	2.66%	0.238%
52	13.625	1024	1027	1029	rVV2	119448	204524	4.22%	0.376%
53	13.660	1029	1030	1031	rVV	66828	81821	1.69%	0.151%
54	13.728	1034	1036	1038	rVV	122462	132218	2.73%	0.243%
55	13.854	1044	1047	1053	rVV2	1369930	2425791	50.01%	4.463%
56	13.968	1055	1057	1059	rVB	72502	82198	1.69%	0.151%
57	14.037	1059	1063	1065	rBV4	50119	135584	2.80%	0.249%
58	14.082	1065	1067	1068	rVV2	47430	57767	1.19%	0.106%
59	14.105	1068	1069	1072	rVB	40706	48516	1.00%	0.089%
60	14.254	1079	1082	1084	rBV	87690	116487	2.40%	0.214%
61	14.322	1086	1088	1091	rVV3	44125	88771	1.83%	0.163%
62	14.380	1091	1093	1096	rVB2	35086	58983	1.22%	0.109%
63	14.597	1109	1112	1114	rBV4	64132	101850	2.10%	0.187%
64	14.665	1116	1118	1120	rVB	70307	76700	1.58%	0.141%
65	14.745	1122	1125	1130	rVB3	39762	81104	1.67%	0.149%
66	14.871	1134	1136	1143	rBV	436128	843867	17.40%	1.553%
67	14.974	1143	1145	1148	rVB	70594	74732	1.54%	0.137%
68	15.145	1158	1160	1163	rBV	227953	263782	5.44%	0.485%
69	15.203	1163	1165	1167	rVV	335537	404827	8.35%	0.745%
70	15.260	1167	1170	1181	rVB	651155	1236997	25.50%	2.276%
71	15.614	1199	1201	1203	rBV	44323	59458	1.23%	0.109%

LSC Area Percent Report

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Data File : BF093718.D
Acq On : 16 Mar 2017 20:46
Operator : SJ/MA
Sample : I2266-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP6

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-BF030717.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	16.048	1237	1239	1246	rVB3	51727	132396	2.73%	0.244%
73	16.265	1255	1258	1262	rBV5	16908	57121	1.18%	0.105%
74	16.563	1280	1284	1285	rBV3	39181	91533	1.89%	0.168%
75	16.608	1285	1288	1292	rVB	119765	255996	5.28%	0.471%
76	16.757	1298	1301	1304	rBV	35037	74973	1.55%	0.138%
77	17.008	1320	1323	1332	rVB	117833	277710	5.73%	0.511%
78	17.157	1332	1336	1342	rBV2	33299	98326	2.03%	0.181%
79	17.260	1342	1345	1349	rBV	19386	55183	1.14%	0.102%

Sum of corrected areas: 54354384

Data Path : Z:\HPCHEM1\BNA F\Data\BF031617\
Data File : BF093718.D
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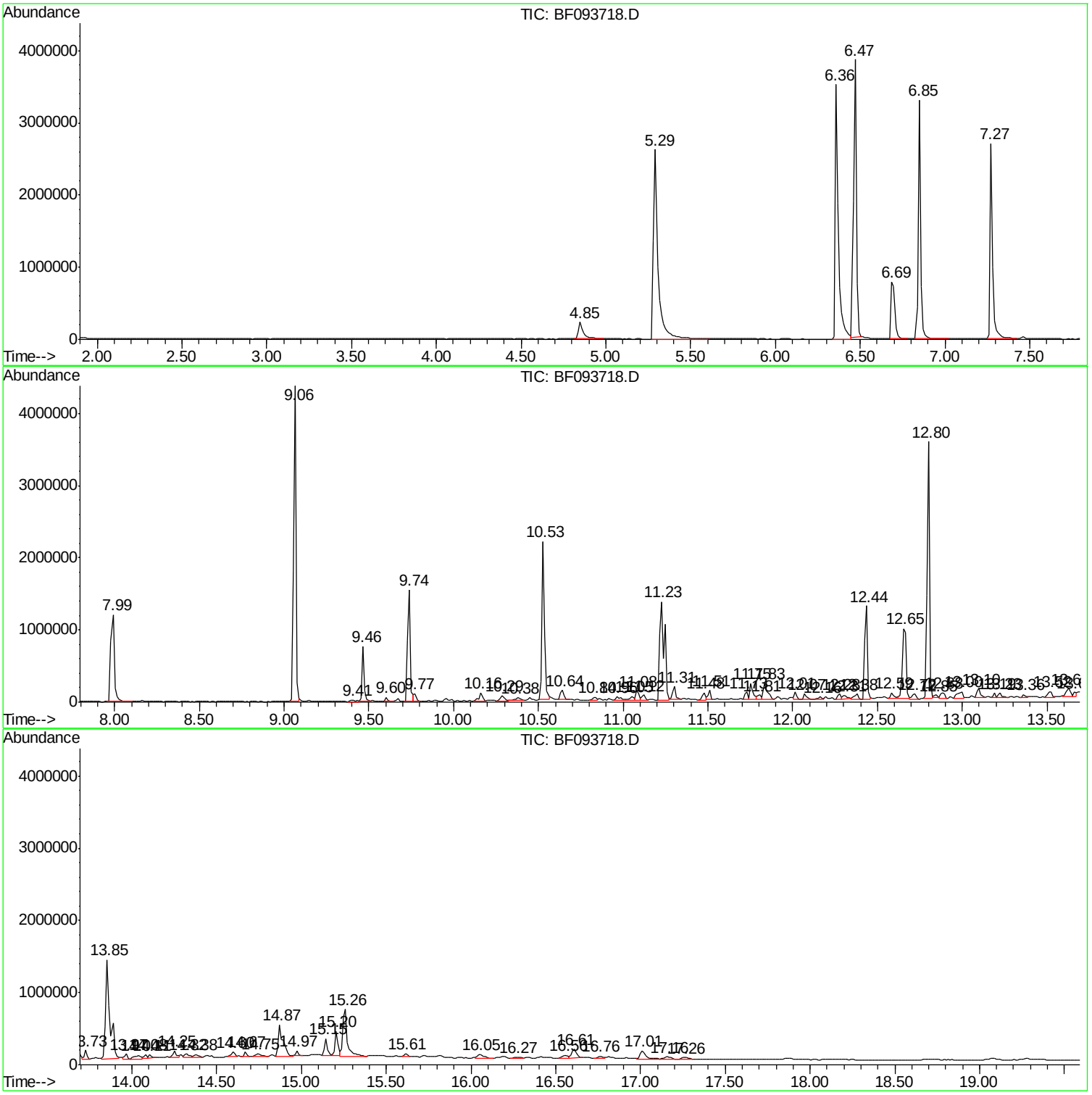
Operator : SJ/MA
Sample : I2266-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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\BF031617\
Data File : BF093718.D
Acq On : 16 Mar 2017 20:46
Operator : SJ/MA
Sample : I2266-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

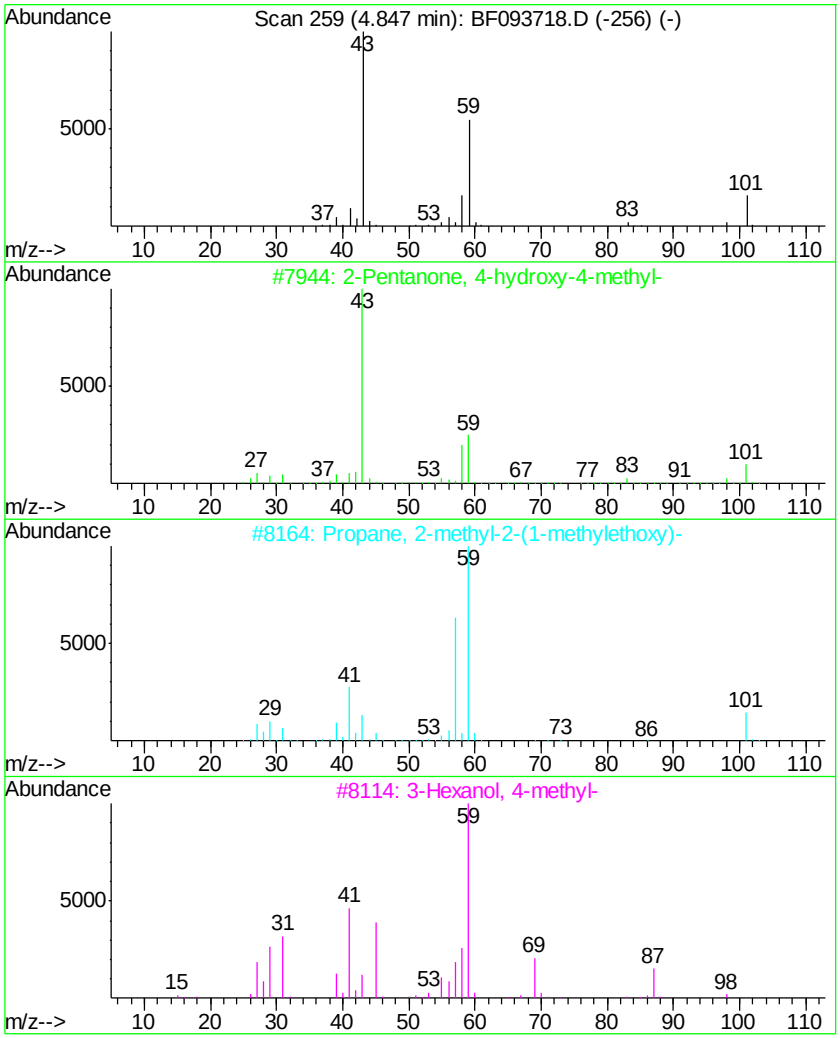
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

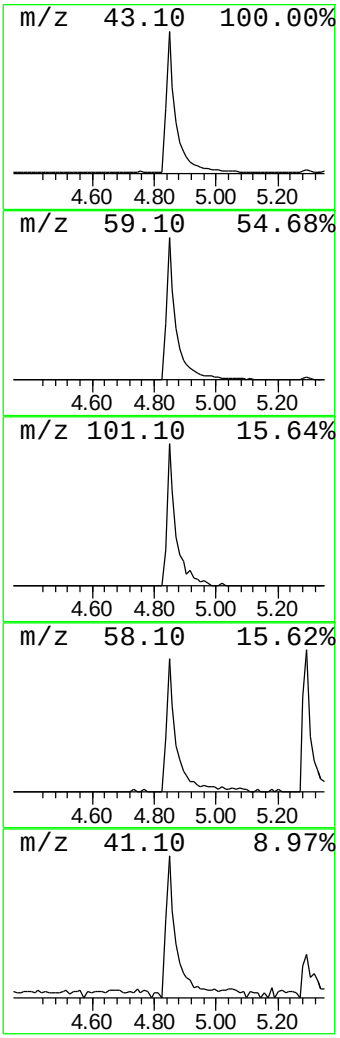
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	8.44 ng	504857	1,4-Dichlorobenzene-d4	6.70

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	53
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28





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Data File : BF093718.D
Acq On : 16 Mar 2017 20:46
Operator : SJ/MA
Sample : I2266-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

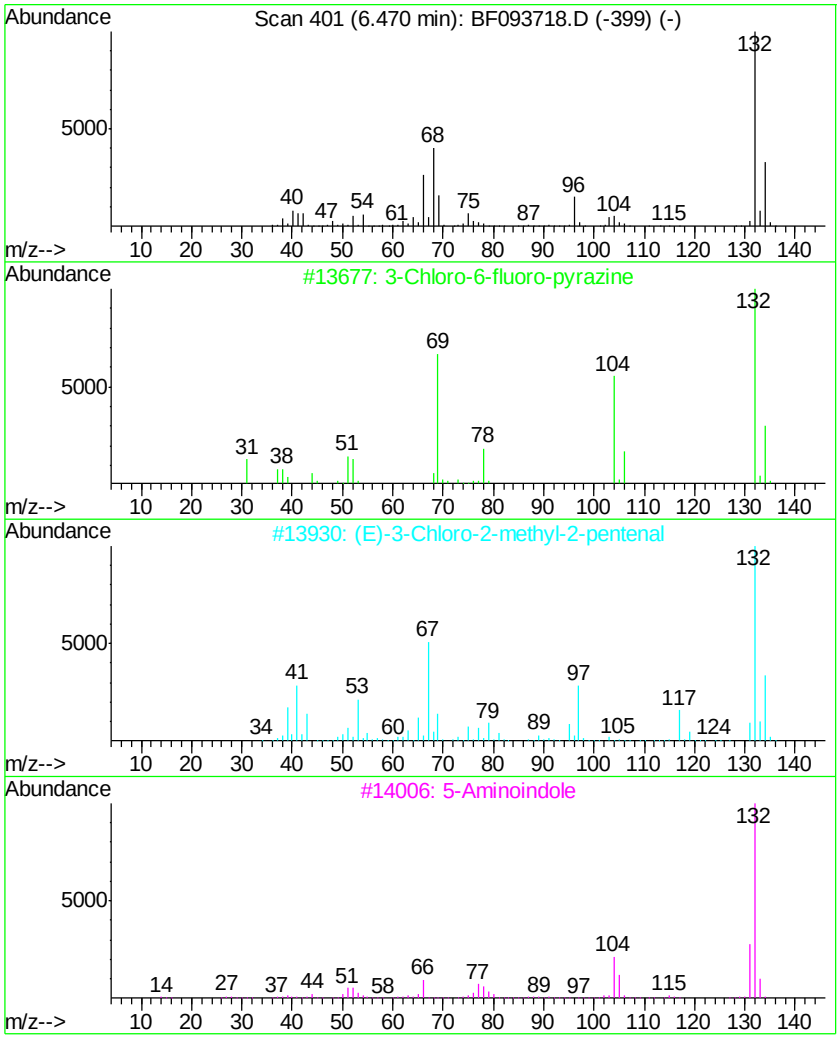
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

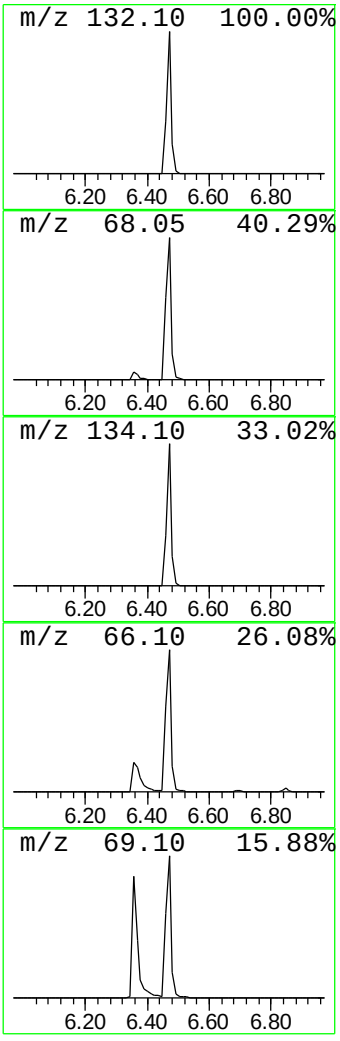
****

Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	74.89 ng	4479500	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9





Data Path : Z:\HPCHEM1\BNA F\Data\BF031617\
Data File : BF093718.D
Acq On : 16 Mar 2017 20:46
Operator : SJ/MA
Sample : I2266-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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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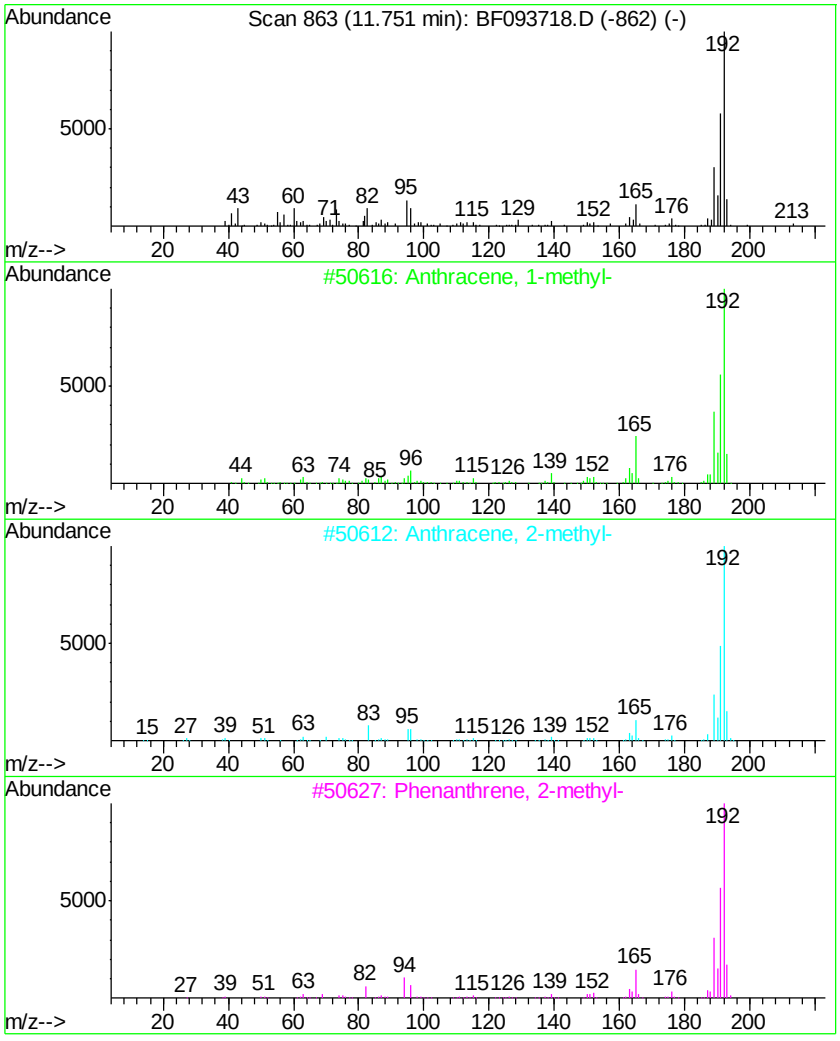
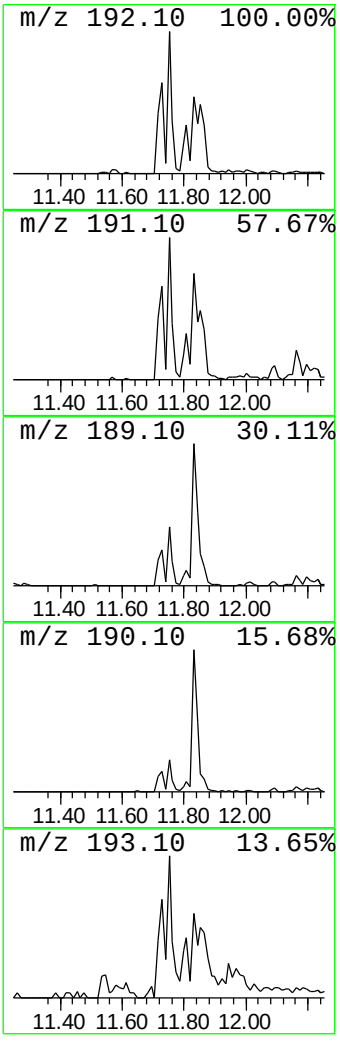
Peak Number 4 Anthracene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	2.06 ng	286799	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	95
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	90
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	90
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	87





Data Path : Z:\HPCHEM1\BNA F\Data\BF031617\
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Sample : I2266-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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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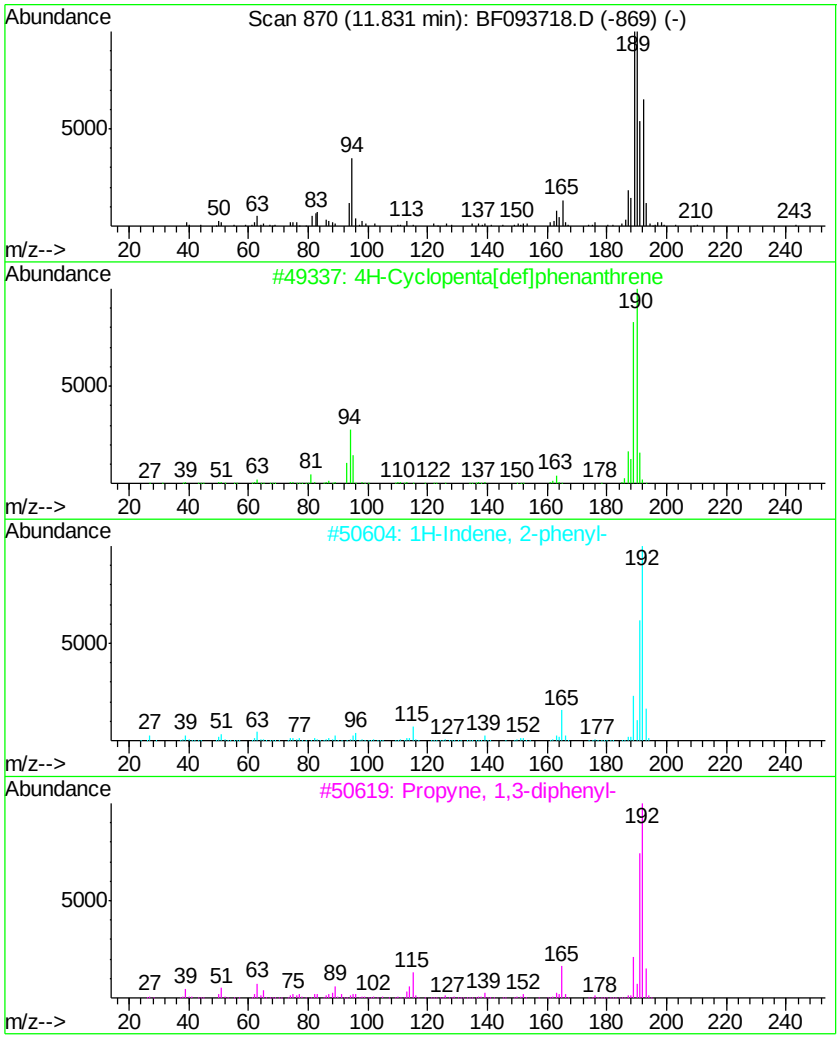
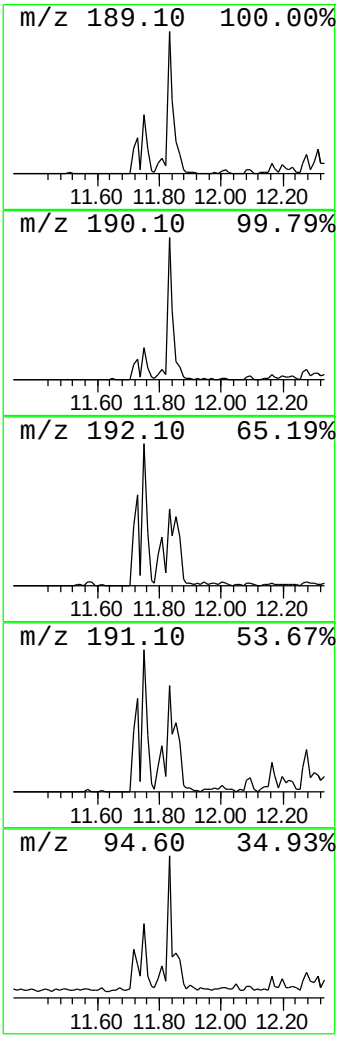
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.83	2.36 ng	328994	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	38
3	Propyne, 1,3-diphenyl-	192	C15H12	004980-70-5	30
4	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	25
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	25





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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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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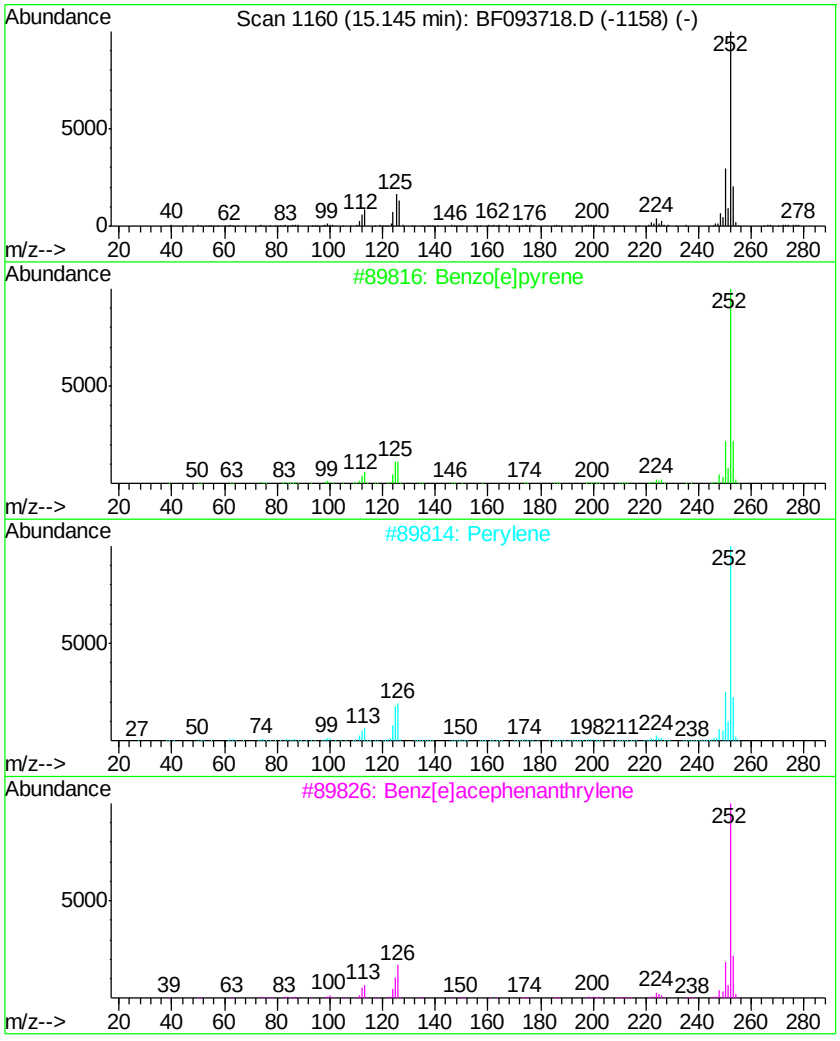
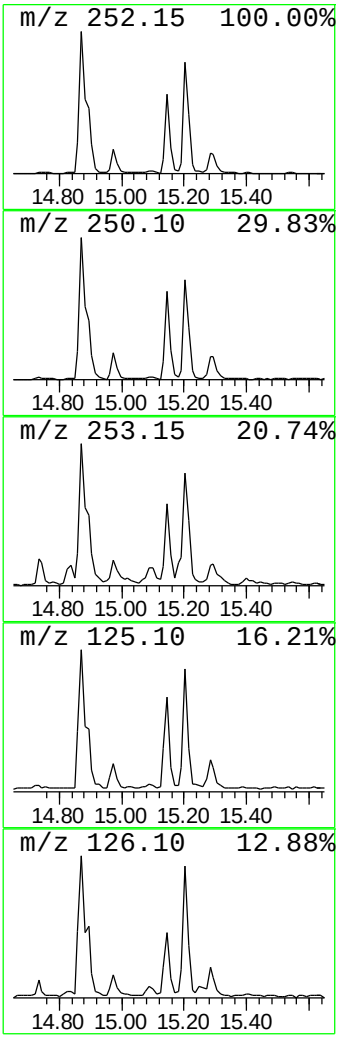
Peak Number 6 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.15	4.26 ng	263782	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	97
2	Perylene	252	C20H12	000198-55-0	94
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	94
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	89





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Data File : BF093718.D
Acq On : 16 Mar 2017 20:46
Operator : SJ/MA
Sample : I2266-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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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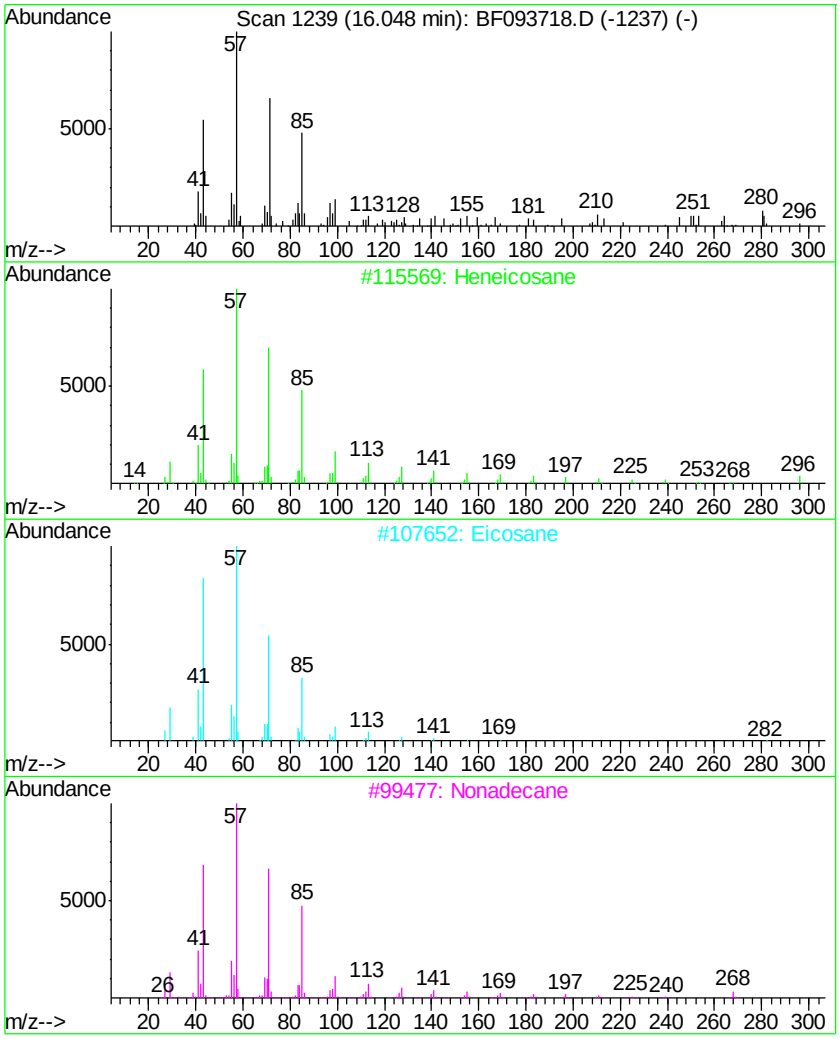
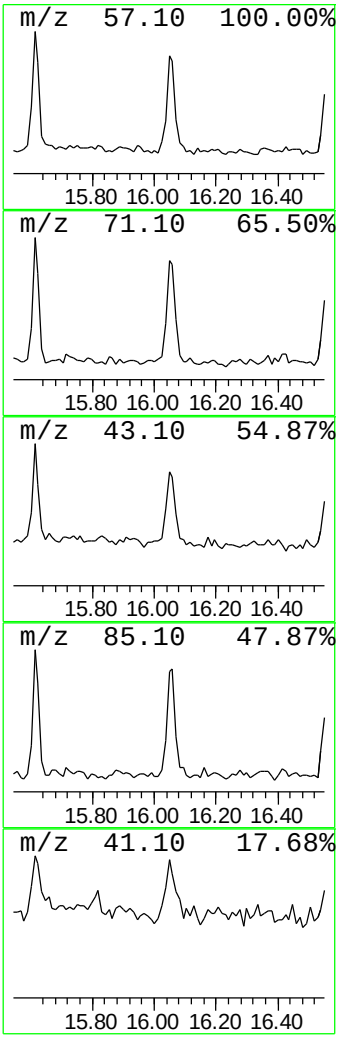
Peak Number 7 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.05	2.14 ng	132396	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	86
2	Eicosane	282	C20H42	000112-95-8	70
3	Nonadecane	268	C19H40	000629-92-5	58
4	5,15-Dimethylnonadecane	296	C21H44	1000131-09-1	53
5	Borane, diethyl(decyloxy)-	226	C14H31BO	1000152-34-3	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\Data\BF031617\
Data File : BF093718.D
Acq On : 16 Mar 2017 20:46
Operator : SJ/MA
Sample : I2266-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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...	4.85	8.4	ng	504857	1	6.70	1196340	20.0
unknown6.47	6.47	74.9	ng	4479500	1	6.70	1196340	20.0
Anthracene, 1-met...	11.75	2.1	ng	286799	4	11.23	2787930	20.0
4H-Cyclopenta[def...	11.83	2.4	ng	328994	4	11.23	2787930	20.0
Benzo[e]pyrene	15.15	4.3	ng	263782	6	15.26	1237000	20.0
Heneicosane	16.05	2.1	ng	132396	6	15.26	1237000	20.0