LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030416\
Data File : BF085247.D
Acq On : 5 Mar 2016 11:52
Operator : SJ/IZ
Sample : H1675-05 5X
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-003(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-BF030316.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	5.156	249	251	256	rBV	156705	150470	15.87%	0.862%
2	5.567	284	287	289	rBV	734823	706569	74.52%	4.048%
3	6.584	373	376	378	rBV	881281	761463	80.31%	4.363%
4	6.733	386	389	391	rBV	899842	778857	82.14%	4.463%
5	6.973	407	410	412	rBV	115785	129218	13.63%	0.740%
6	7.122	421	423	426	rVB	656636	604520	63.75%	3.464%
7	7.247	430	434	436	rBV2	5908	10565	1.11%	0.061%
8	7.522	456	458	461	rVB	375922	417446	44.03%	2.392%
9	8.253	520	522	523	rBV	205035	167404	17.65%	0.959%
10	8.276	523	524	526	rVB	39162	31866	3.36%	0.183%
11	8.962	583	584	586	rVB2	18721	22899	2.42%	0.131%
12	9.065	591	593	595	rBV	20840	17773	1.87%	0.102%
13	9.328	614	616	618	rBV	1068055	853202	89.98%	4.888%
14	9.408	622	623	627	rVB	15347	21933	2.31%	0.126%
15	9.590	637	639	641	rVB	14184	16852	1.78%	0.097%
16	9.670	643	646	649	rBV2	22290	33725	3.56%	0.193%
17	9.716	649	650	653	rBV	58634	71538	7.54%	0.410%
18	9.876	661	664	666	rBV	40374	60196	6.35%	0.345%
19	9.945	666	670	671	rVV2	16935	33850	3.57%	0.194%
20	10.013	671	676	677	rVV2	183501	184371	19.44%	1.056%
21	10.048	677	679	680	rVB	45823	55357	5.84%	0.317%
22	10.173	687	690	691	rBV2	6262	12202	1.29%	0.070%
23	10.208	691	693	696	rVB	33023	46012	4.85%	0.264%
24	10.253	696	697	699	rBV	13515	14597	1.54%	0.084%
25	10.413	709	711	712	rBV	9796	10518	1.11%	0.060%
26	10.436	712	713	715	rVB	46439	35984	3.79%	0.206%
27	10.551	722	723	726	rBV	26588	39100	4.12%	0.224%
28	10.665	726	733	736	rBV4	16417	51770	5.46%	0.297%
29	10.711	736	737	739	rVB	15479	11762	1.24%	0.067%
30	10.791	742	744	747	rBV	234265	253451	26.73%	1.452%
31	10.916	753	755	758	rBV2	36283	67972	7.17%	0.389%
32	11.099	767	771	773	rBV3	11228	25558	2.70%	0.146%
33	11.236	780	783	784	rBV	11098	18055	1.90%	0.103%
34	11.293	787	788	790	rVV	32629	38351	4.04%	0.220%

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Misc :
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Instrument : BNA_F
ClientSampleId : SP-003(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

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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.362	790	794	795	rVV2	30357	49002	5.17%	0.281%
36	11.396	795	797	799	rVB3	27768	38170	4.03%	0.219%
37	11.522	804	808	810	rBV2	433998	579887	61.16%	3.322%
38	11.568	810	812	814	rVV	236585	204957	21.62%	1.174%
39	11.602	814	815	817	rVB	20527	16468	1.74%	0.094%
40	11.671	817	821	823	rVB3	10950	17280	1.82%	0.099%
41	11.716	823	825	828	rBV2	59983	91133	9.61%	0.522%
42	11.785	829	831	833	rVV	23574	27193	2.87%	0.156%
43	11.831	833	835	836	rVB2	8015	11625	1.23%	0.067%
44	11.945	844	845	847	rBV2	10062	14114	1.49%	0.081%
45	11.991	847	849	850	rVV	45833	59380	6.26%	0.340%
46	12.025	850	852	854	rVV	100482	113106	11.93%	0.648%
47	12.071	854	856	857	rVV	43778	43622	4.60%	0.250%
48	12.105	857	859	863	rVV	94299	153219	16.16%	0.878%
49	12.196	863	867	868	rVV3	25315	45565	4.81%	0.261%
50	12.231	868	870	871	rVV3	13153	19131	2.02%	0.110%
51	12.311	873	877	879	rVB2	82669	137739	14.53%	0.789%
52	12.436	886	888	889	rBV2	23252	28564	3.01%	0.164%
53	12.494	889	893	896	rVV4	30804	52760	5.56%	0.302%
54	12.539	896	897	899	rBV	40845	56356	5.94%	0.323%
55	12.574	899	900	903	rBV2	30847	58263	6.14%	0.334%
56	12.631	903	905	907	rVB	64691	61611	6.50%	0.353%
57	12.676	907	909	910	rBV2	16932	21729	2.29%	0.124%
58	12.711	910	912	914	rVB	913530	869207	91.67%	4.980%
59	12.768	914	917	918	rBV2	32435	61333	6.47%	0.351%
60	12.802	918	920	921	rBV	31743	27097	2.86%	0.155%
61	12.859	921	925	929	rBV5	44035	116703	12.31%	0.669%
62	12.939	929	932	934	rBV	809705	948197	100.00%	5.433%
63	12.985	934	936	939	rVB2	37134	52775	5.57%	0.302%
64	13.076	940	944	948	rBV	687373	742264	78.28%	4.253%
65	13.156	948	951	952	rBV2	58471	111312	11.74%	0.638%
66	13.259	957	960	962	rVV	98824	201160	21.22%	1.153%
67	13.328	964	966	967	rVB	84190	79603	8.40%	0.456%
68	13.362	967	969	971	rBV	66108	78411	8.27%	0.449%
69	13.465	976	978	979	rBV	40232	57177	6.03%	0.328%
70	13.762	1002	1004	1007	rVB	97480	117842	12.43%	0.675%
71	13.877	1012	1014	1016	rBV2	91719	159941	16.87%	0.916%

LSC Area Percent Report

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Sample : H1675-05 5X
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-003(0-2)

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
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Start Thrs: 0.2 Max Peaks: 100
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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	13.934	1018	1019	1021	rVV2	53591	90671	9.56%	0.520%
73	13.968	1021	1022	1025	rVB	96973	137900	14.54%	0.790%
74	14.128	1033	1036	1037	rBV2	368383	619152	65.30%	3.547%
75	14.162	1037	1039	1042	rVB2	292432	440432	46.45%	2.523%
76	14.517	1068	1070	1072	rBV	68809	76053	8.02%	0.436%
77	14.860	1096	1100	1103	rVB5	149941	392125	41.35%	2.247%
78	15.180	1125	1128	1131	rBV	360388	781816	82.45%	4.479%
79	15.477	1152	1154	1157	rVB	206292	288050	30.38%	1.650%
80	15.534	1157	1159	1163	rVV	190860	321183	33.87%	1.840%
81	15.602	1163	1165	1166	rVV	96111	121704	12.84%	0.697%
82	15.637	1166	1168	1171	rVB2	118692	192404	20.29%	1.102%
83	17.077	1291	1294	1297	rBV2	102523	215909	22.77%	1.237%
84	17.523	1330	1333	1342	rVB	79703	187736	19.80%	1.076%
85	18.311	1401	1402	1404	rVB2	62087	47039	4.96%	0.270%
86	18.563	1422	1424	1426	rBV3	116155	120823	12.74%	0.692%
87	18.654	1430	1432	1433	rVB2	35029	39274	4.14%	0.225%
88	18.803	1444	1445	1447	rBV2	64136	75120	7.92%	0.430%
89	18.894	1450	1453	1455	rBV4	59442	146876	15.49%	0.842%
90	18.928	1455	1456	1461	rVB3	81811	174200	18.37%	0.998%
91	18.997	1461	1462	1464	rBV	210337	155526	16.40%	0.891%
92	19.100	1470	1471	1472	rBV	24214	22427	2.37%	0.128%
93	19.146	1472	1475	1476	rVV3	41356	64471	6.80%	0.369%
94	19.169	1476	1477	1478	rVB	87176	59759	6.30%	0.342%
95	19.260	1483	1485	1487	rBV	48762	44512	4.69%	0.255%
96	19.306	1487	1489	1490	rBV2	102928	105807	11.16%	0.606%
97	19.351	1492	1493	1497	rVV4	122103	236598	24.95%	1.356%
98	19.420	1497	1499	1500	rVV2	102830	133076	14.03%	0.762%
99	19.454	1500	1502	1505	rVB4	533678	858112	90.50%	4.917%
100	19.511	1505	1507	1508	rBV2	20769	25278	2.67%	0.145%

Sum of corrected areas: 17453335

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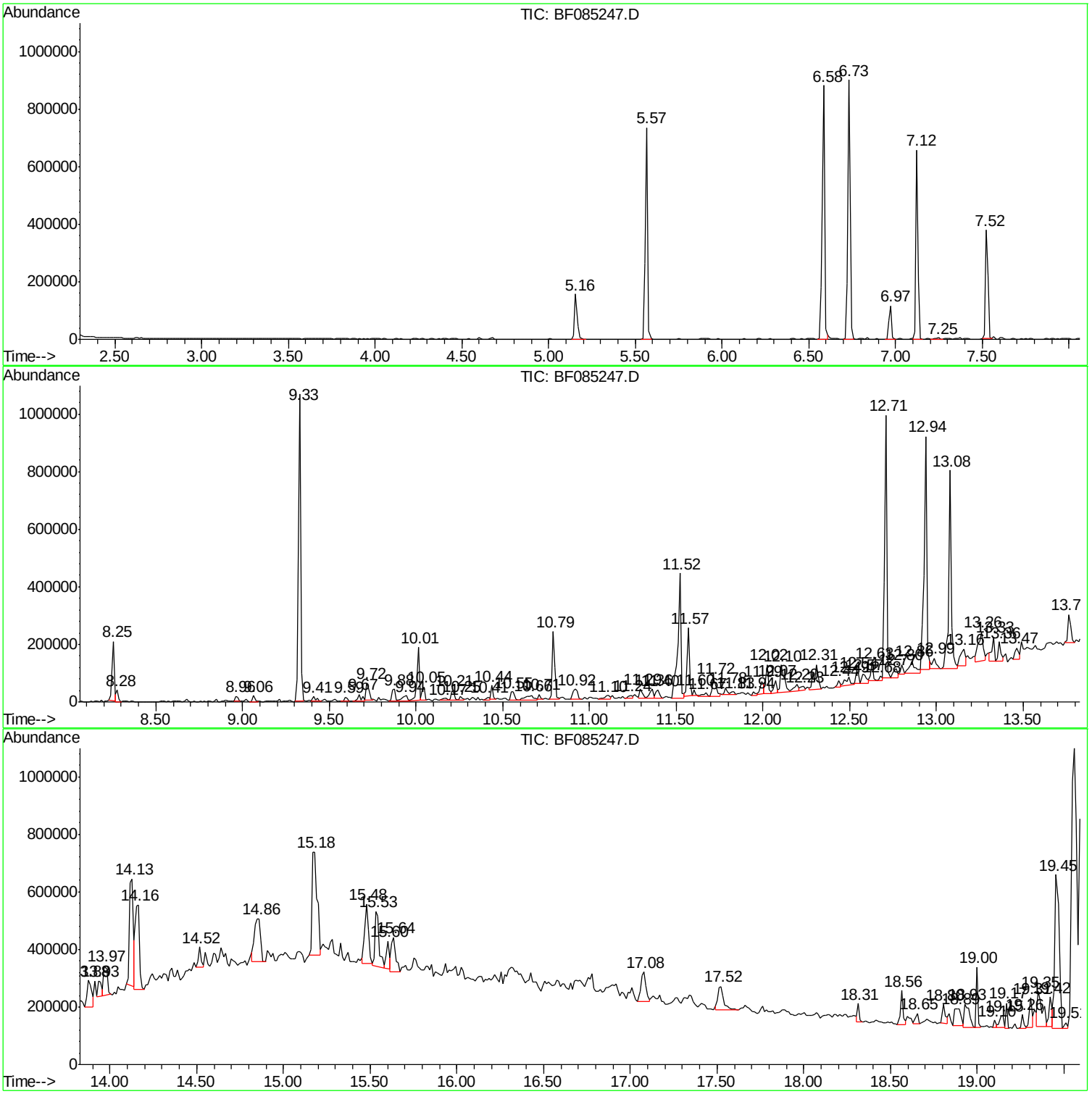
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-003(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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Instrument : BNA_F
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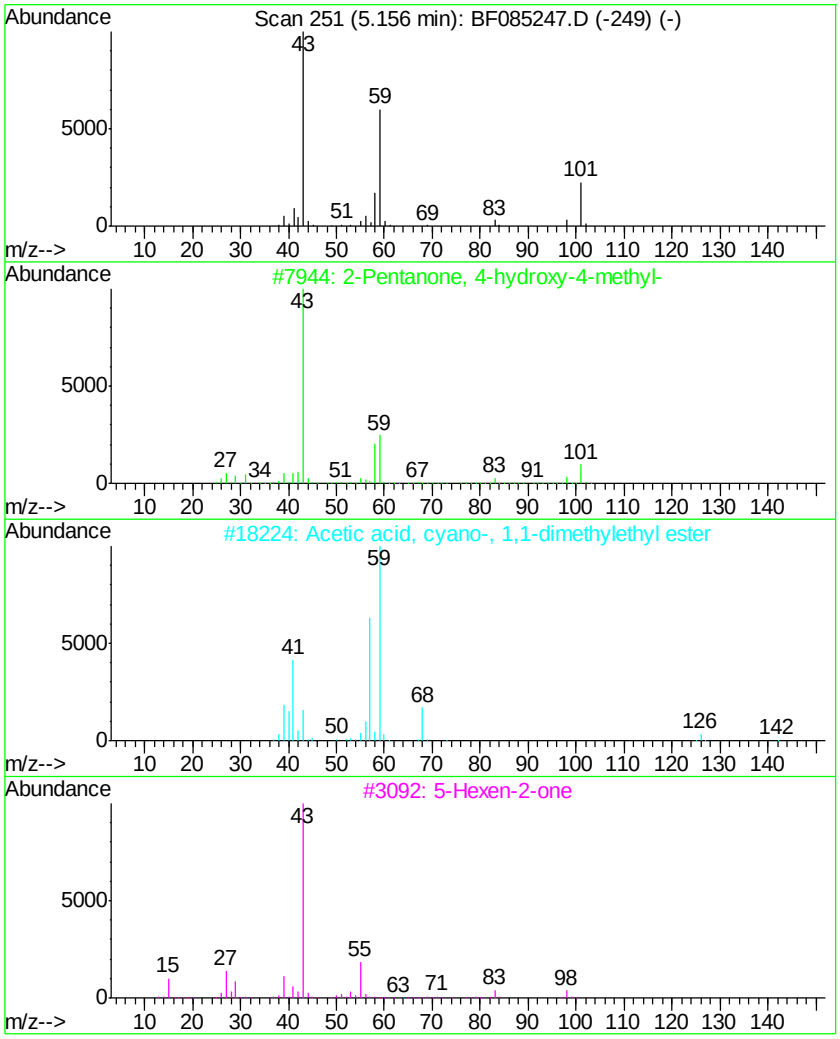
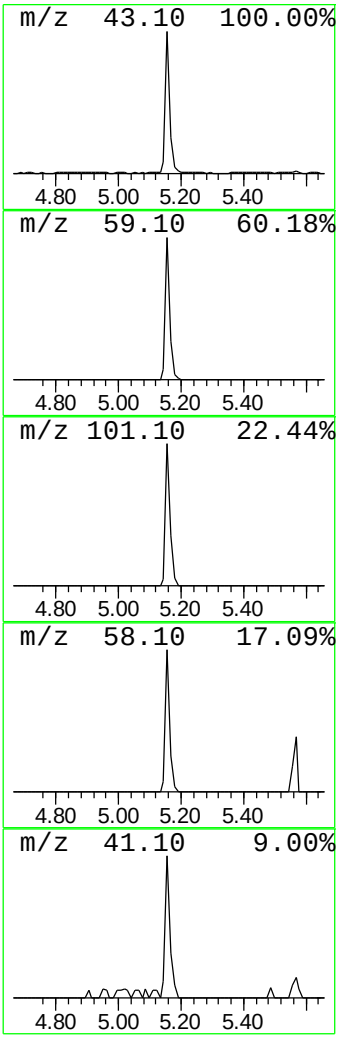
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	23.29 ng	150470	1,4-Dichlorobenzene-d4	6.97

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	17
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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Instrument : BNA_F
ClientSampleId : SP-003(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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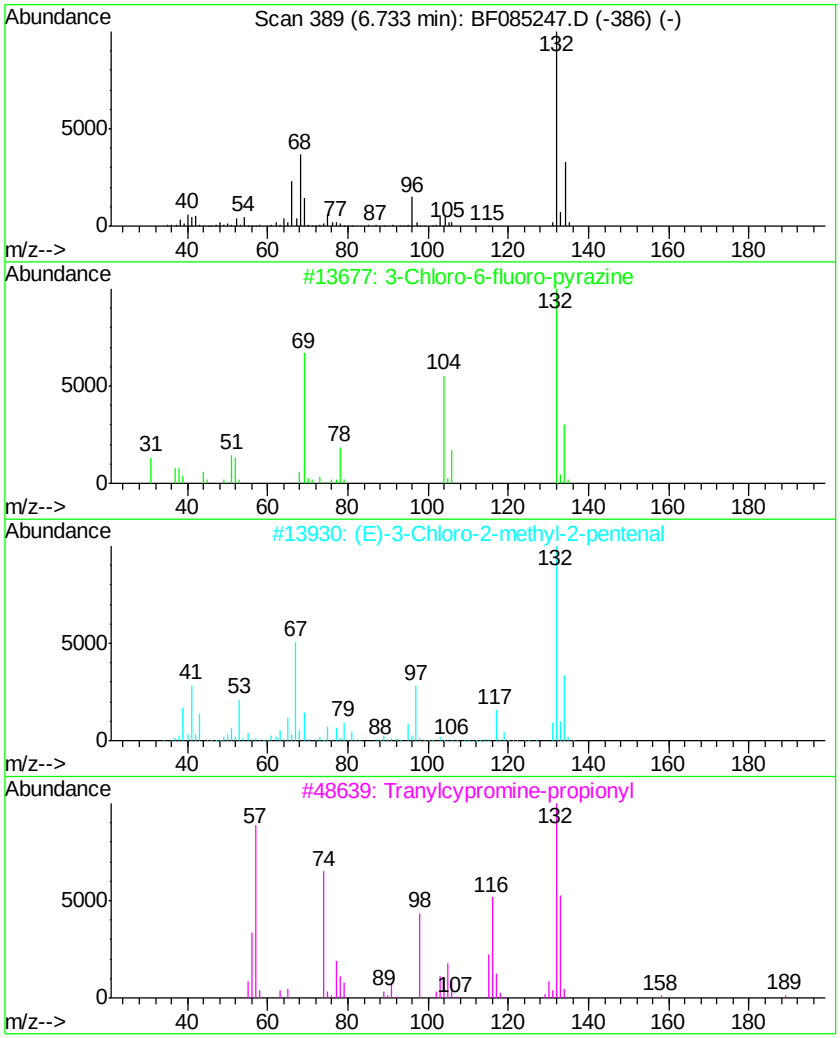
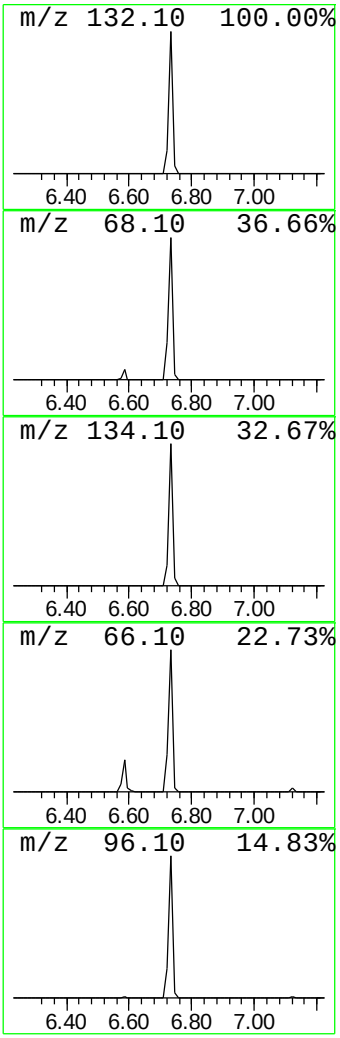
****

Peak Number 2 unknown6.73 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	120.55 ng	778857	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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

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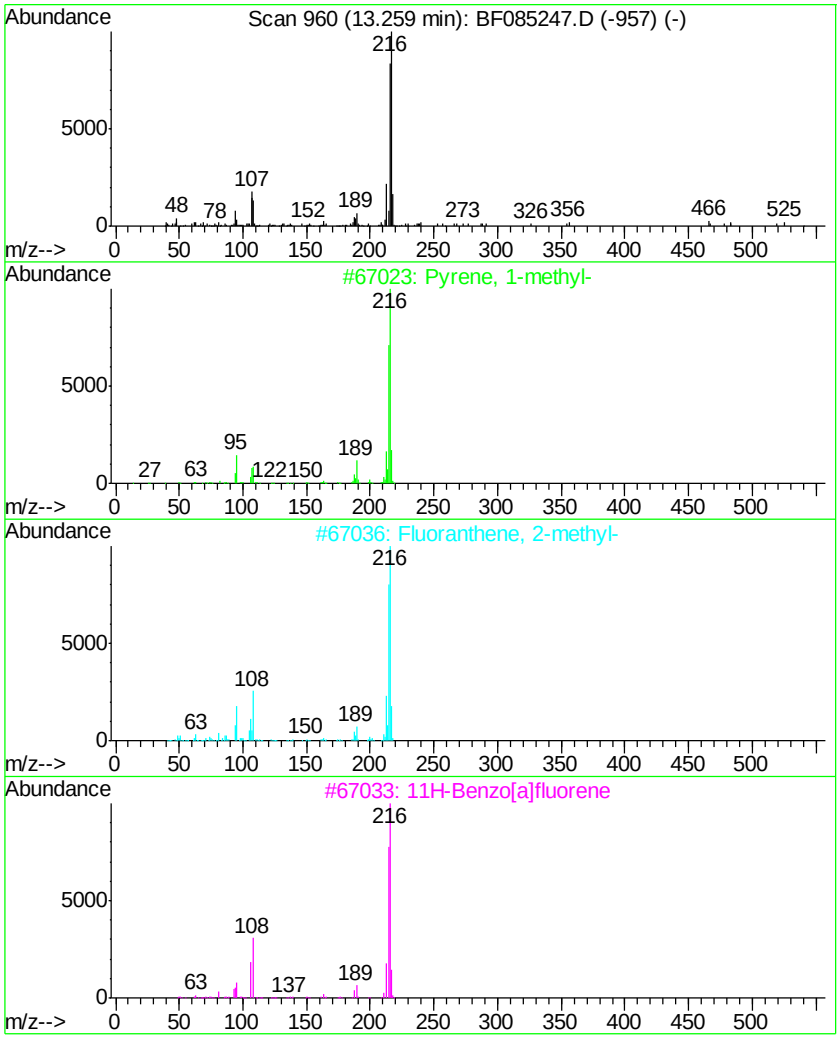
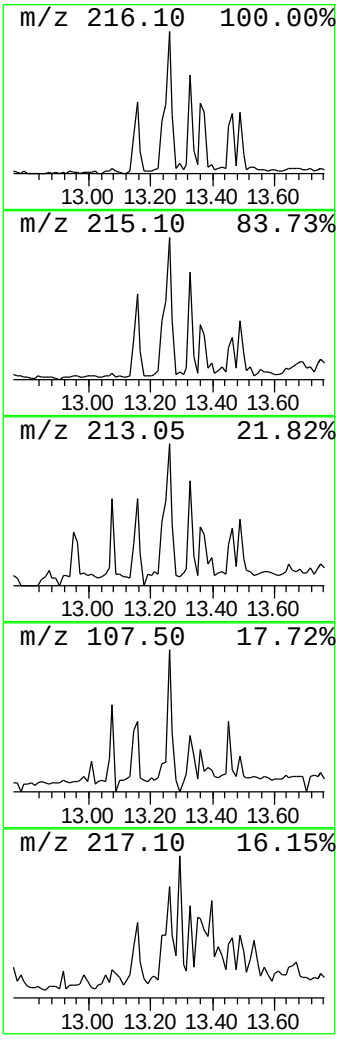
Peak Number 4 Pyrene, 1-methyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.26	6.50 ng	201160	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
2	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	90
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90
4	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	81





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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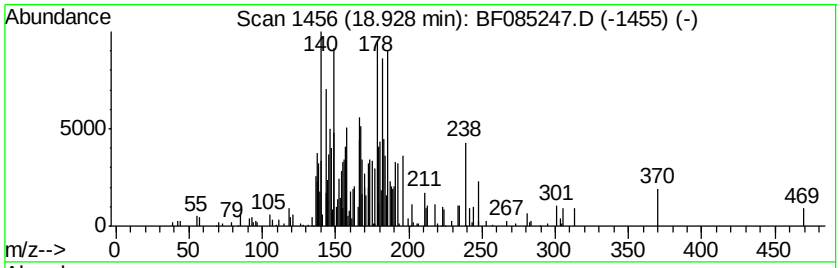
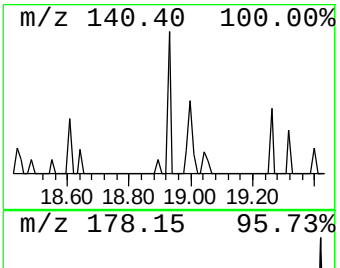
Peak Number 12 unknown18.93 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.93	28.63 ng	174200	Perylene-d12	15.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2-Carbamoylethyl)-2,3-dihydro...	183	C7H9N3O3	031535-00-9	25
2	3-Bromobenzoic acid hydrazide	214	C7H7BrN2O	039115-96-3	14
3	Isobenzofuran-1(3H)-one, 5-bromo-	212	C8H5BrO2	064169-34-2	10
4	Pyridine, 2-(2-phenylethyl)-	183	C13H13N	002116-62-3	10
5	1,3,5-Triazine, 2,4,6-trichloro-	183	C3Cl3N3	000108-77-0	10





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Sample : H1675-05 5X
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-003(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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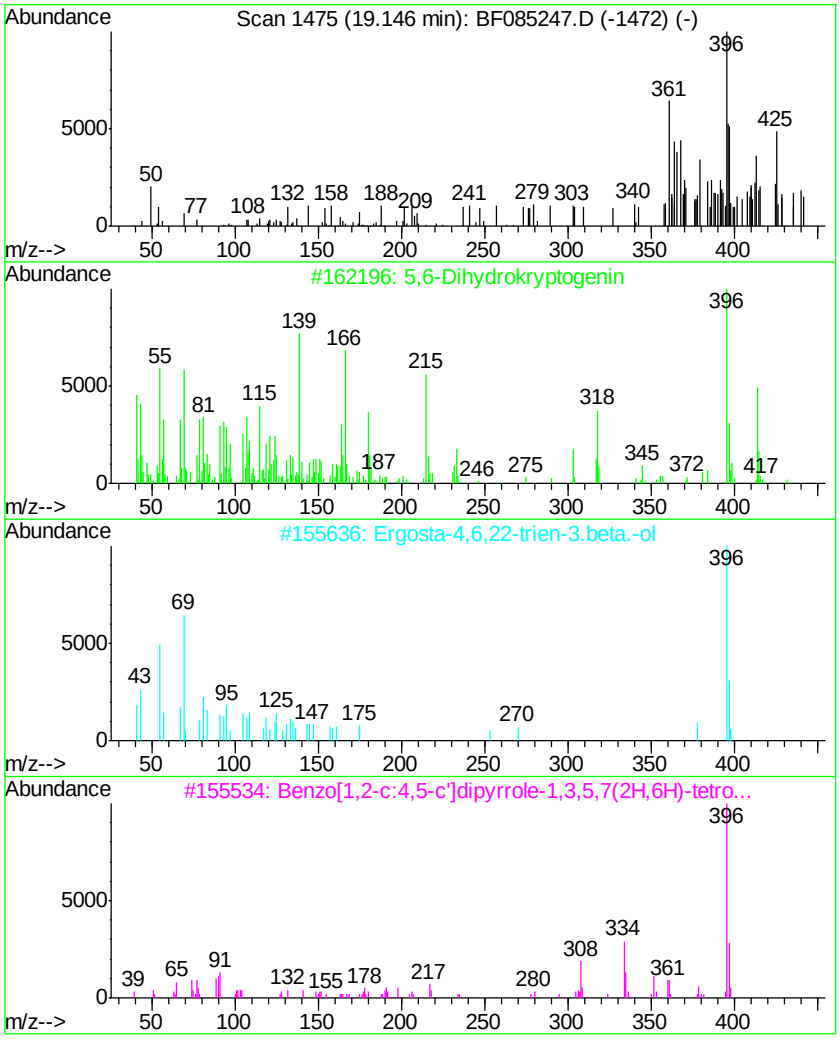
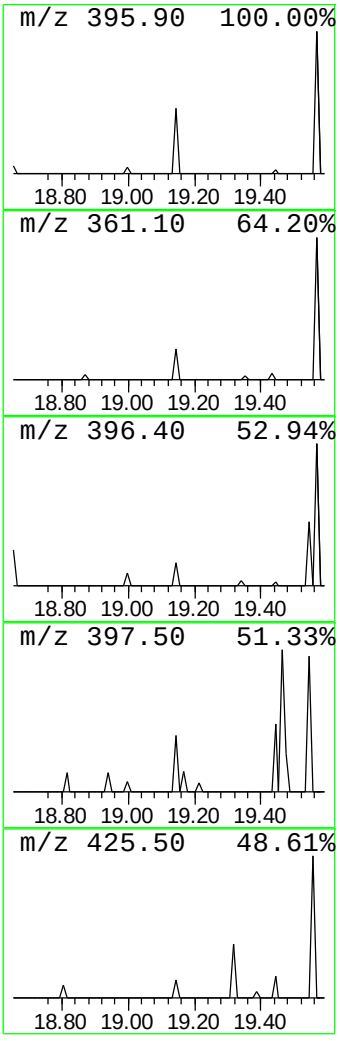
Peak Number 14 unknown19.15 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.15	10.59 ng	64471	Perylene-d12	15.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,6-Dihydrokryptogenin	432	C27H44O4	122386-94-1	25
2	Ergosta-4,6,22-trien-3.beta.-ol	396	C28H44O	034026-93-2	22
3	Benzo[1,2-c:4,5-c']dipyrrole-1,3...	396	C24H16N2O4	031663-73-7	22
4	2,4-Imidazolidinedione, 1,3-diet...	396	C22H28N2O3Si	057326-25-7	22
5	Spiro[7H-indeno[4,5-d]-1,3-dioxo...	439	C24H25NO7	030833-09-1	12





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030416\
Data File : BF085247.D
Acq On : 5 Mar 2016 11:52
Operator : SJ/IZ
Sample : H1675-05 5X
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-003(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

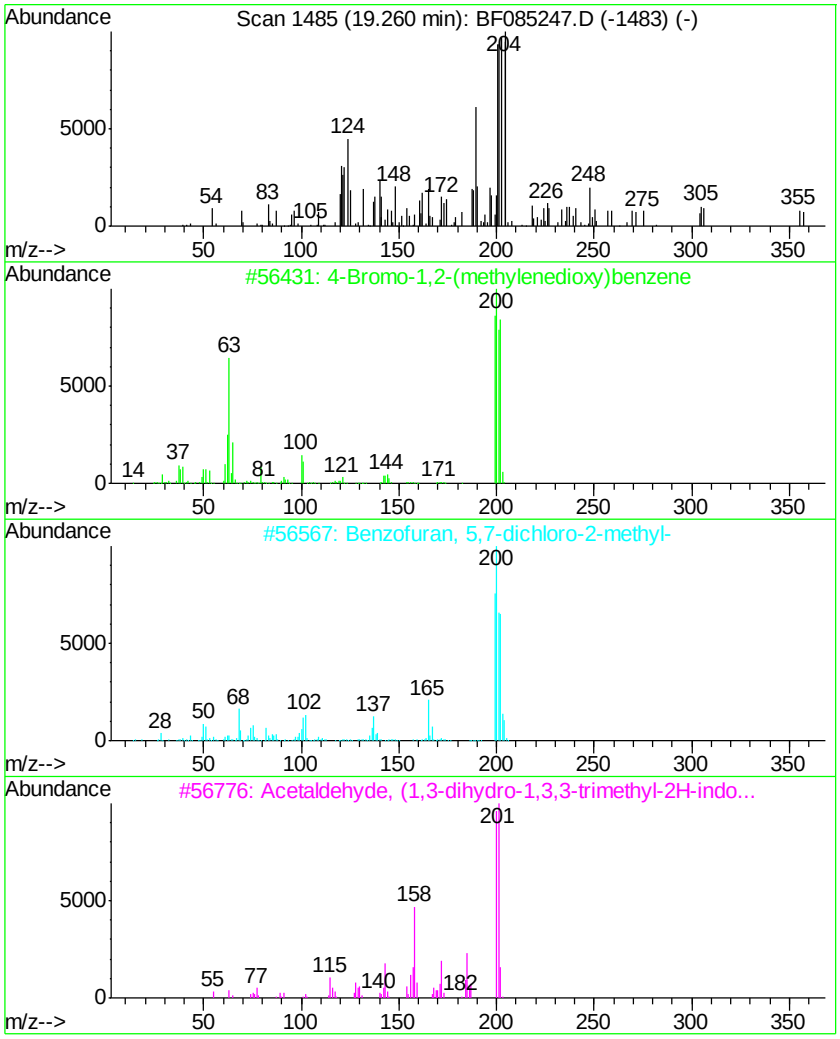
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

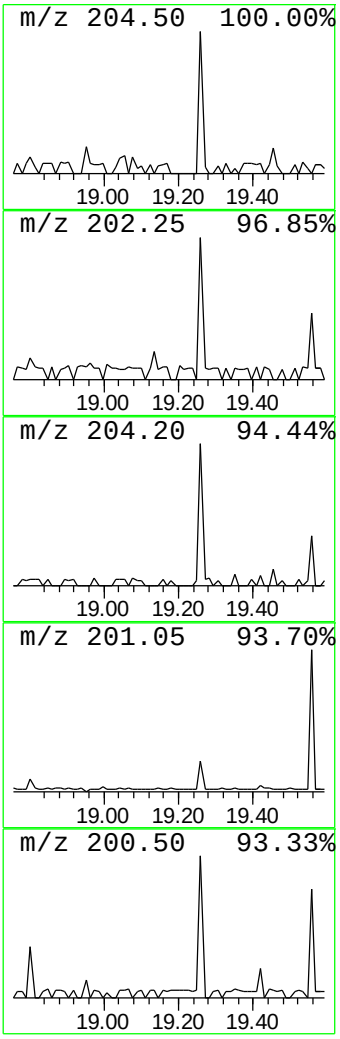
****

Peak Number 16 unknown19.26 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.26	7.31 ng	44512	Perylene-d12	15.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Bromo-1,2-(methylenedioxy)benzene	200	C7H5BrO2	002635-13-4	35
2	Benzofuran, 5,7-dichloro-2-methyl-	200	C9H6Cl2O	042969-85-7	32
3	Acetaldehyde, (1,3-dihydro-1,3,3...	201	C13H15NO	000084-83-3	22
4	4-(3-Methylphenylamino)-pyrimidi...	201	C11H11N3O	127970-30-3	22
5	Stannane, triethenylmethyl-	216	C7H12Sn	038178-25-5	18





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Instrument : BNA_F
ClientSampleId : SP-003(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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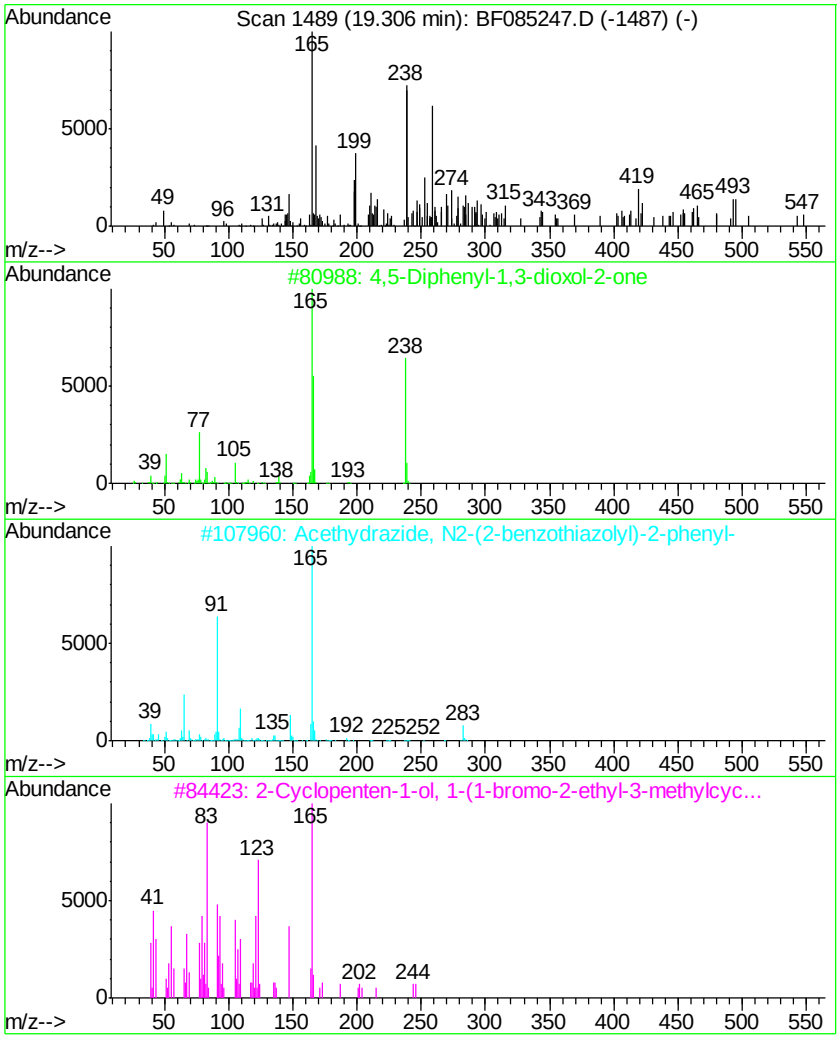
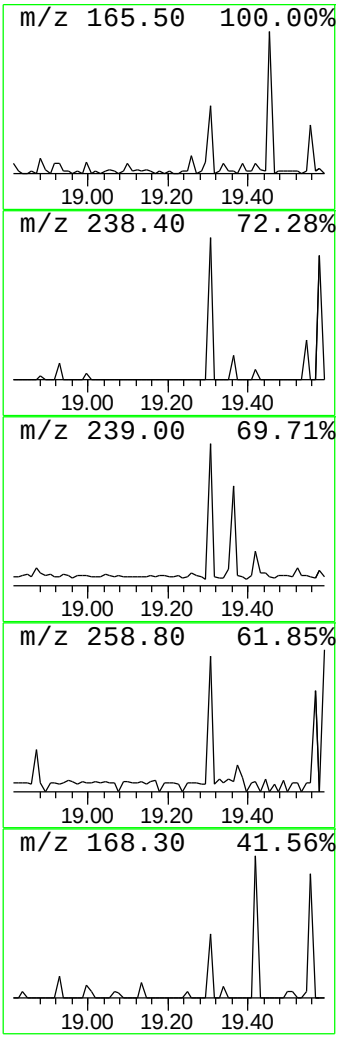
Peak Number 17 unknown19.31 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.31	17.39 ng	105807	Perylene-d12	15.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,5-Diphenyl-1,3-dioxol-2-one	238	C15H10O3	021240-34-6	32
2	Acethydrazide, N2-(2-benzothiazo...	283	C15H13N3OS	311788-35-9	12
3	2-Cyclopenten-1-ol, 1-(1-bromo-2...	244	C11H17BrO	079209-32-8	10
4	2-(3-Chloro-propyl)-benzo(de)iso...	273	C15H12ClNO2	202805-33-2	10
5	8-Hydroxymethyladenine	165	C6H7N5O	030466-95-6	10





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Operator : SJ/IZ
Sample : H1675-05 5X
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-003(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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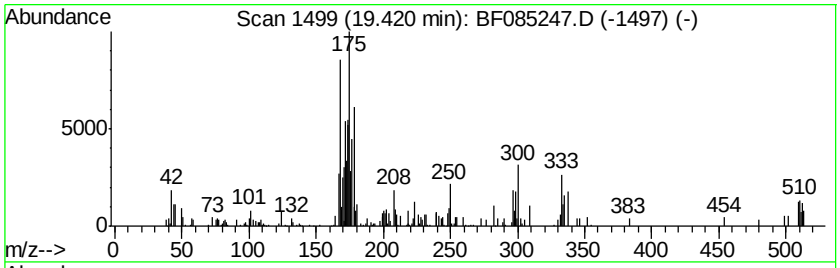
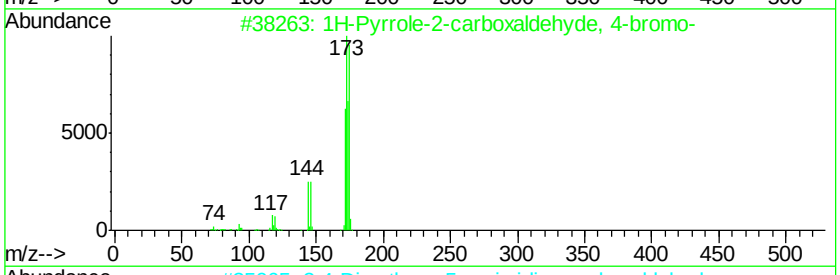
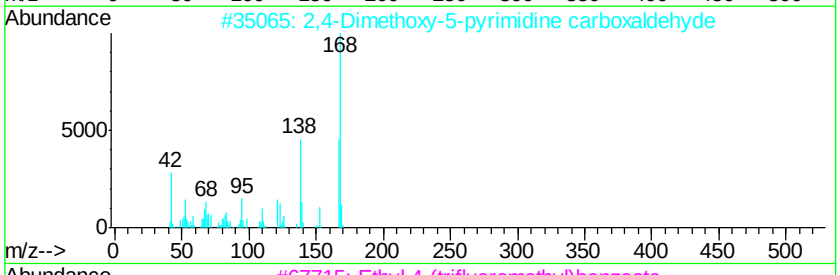
Peak Number 19 unknown19.42 Concentration Rank 10

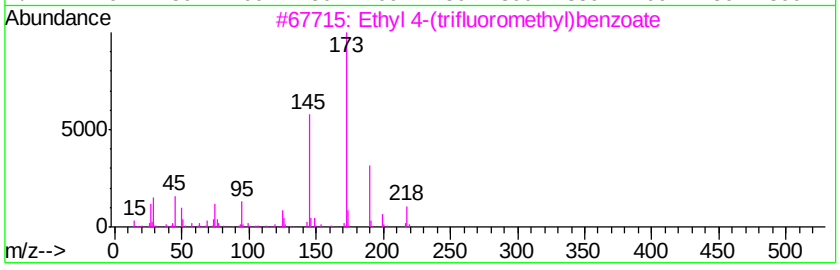
R.T.	EstConc	Area	Relative to ISTD	R.T.
19.42	21.87 ng	133076	Perylene-d12	15.60

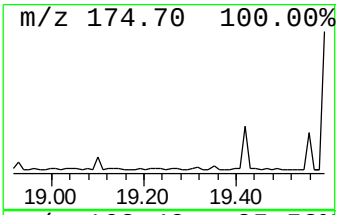
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrrole-2-carboxaldehyde, 4-b...	173	C5H4BrNO	000931-33-9	46
2	2,4-Dimethoxy-5-pyrimidine carbo...	168	C7H8N2O3	052606-02-7	10
3	Ethyl 4-(trifluoromethyl)benzoate	218	C10H9F3O2	000583-02-8	10
4	5-Imidazolic acid, 4-bromo-, eth...	218	C6H7BrN2O2	1000116-73-2	10
5	1-[2-Methoxy-5-nitrophenyl]-3-am...	253	C9H11N5O4	1000255-99-4	9

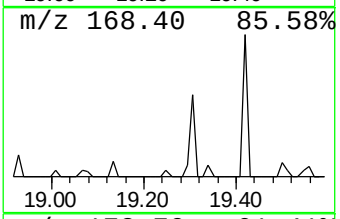


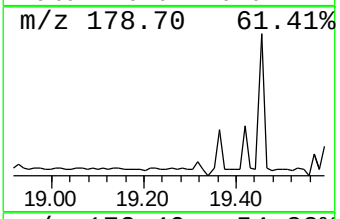


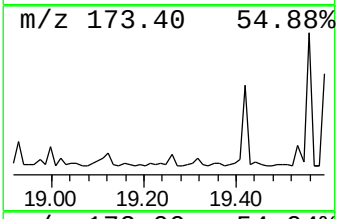


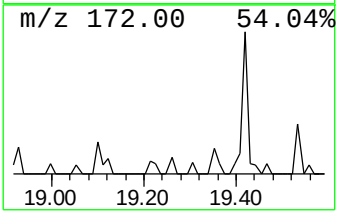












Tentatively Identified Compound (LSC) summary

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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...	5.16	23.3	ng	150470	1	6.97	129218	20.0
unknown6.73	6.73	120.6	ng	778857	1	6.97	129218	20.0
Pyrene, 1-methyl-	13.26	6.5	ng	201160	5	14.13	619152	20.0
unknown18.93	18.93	28.6	ng	174200	6	15.60	121704	20.0
unknown19.15	19.15	10.6	ng	64471	6	15.60	121704	20.0
unknown19.26	19.26	7.3	ng	44512	6	15.60	121704	20.0
unknown19.31	19.31	17.4	ng	105807	6	15.60	121704	20.0
unknown19.42	19.42	21.9	ng	133076	6	15.60	121704	20.0