LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060916\
Data File : BF087856.D
Acq On : 9 Jun 2016 17:00
Operator : UM/SJ
Sample : H3399-01 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-25

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-BF060716.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	1.747	13	14	24	rVB	161838	290252	8.80%	0.972%
2	1.884	24	26	38	rVV	1576424	3296920	100.00%	11.036%
3	2.033	38	39	73	rVB2	87459	462583	14.03%	1.549%
4	4.981	295	297	302	rBV	131691	156994	4.76%	0.526%
5	5.404	332	334	337	rBV	1231264	1187225	36.01%	3.974%
6	6.090	392	394	396	rBV	44491	36590	1.11%	0.122%
7	6.444	423	425	428	rBV	1106496	1135380	34.44%	3.801%
8	6.582	435	437	440	rBV	1487522	1284175	38.95%	4.299%
9	6.822	455	458	460	rBV	838114	807938	24.51%	2.705%
10	6.970	469	471	474	rVB	987726	1011264	30.67%	3.385%
11	7.382	504	507	509	rBV	1022811	881536	26.74%	2.951%
12	8.102	568	570	574	rBV2	1067878	1107472	33.59%	3.707%
13	9.176	662	664	666	rBV	1712623	1404074	42.59%	4.700%
14	9.576	697	699	701	rBV2	58690	83125	2.52%	0.278%
15	9.851	721	723	725	rBV	1212454	1071124	32.49%	3.586%
16	9.885	725	726	728	rVB	185452	130833	3.97%	0.438%
17	10.056	739	741	743	rBV	94207	82954	2.52%	0.278%
18	10.262	755	759	760	rBV	49768	47377	1.44%	0.159%
19	10.399	769	771	773	rBV	113456	128427	3.90%	0.430%
20	10.639	789	792	794	rBV2	548212	743407	22.55%	2.489%
21	10.765	800	803	806	rBV	39634	60469	1.83%	0.202%
22	10.936	815	818	820	rBV2	23125	44276	1.34%	0.148%
23	11.096	827	832	834	rBV4	14563	41166	1.25%	0.138%
24	11.131	834	835	838	rVB	44625	41076	1.25%	0.138%
25	11.222	838	843	848	rBV3	63612	178231	5.41%	0.597%
26	11.325	850	852	854	rBV	661253	1313948	39.85%	4.398%
27	11.359	854	855	856	rVV	858539	590558	17.91%	1.977%
28	11.405	856	859	860	rVB	314513	271111	8.22%	0.908%
29	11.554	869	872	874	rBV2	117602	139608	4.23%	0.467%
30	11.828	894	896	897	rBV	112530	94871	2.88%	0.318%
31	11.851	897	898	900	rVV	100221	129556	3.93%	0.434%
32	11.896	900	902	904	rVV2	85524	92149	2.80%	0.308%
33	11.942	904	906	910	rVB2	199801	263823	8.00%	0.883%
34	12.125	920	922	926	rVB2	94258	125840	3.82%	0.421%

LSC Area Percent Report

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Operator : UM/SJ
Sample : H3399-01 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-25

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
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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.274	932	935	936	rBV2	32647	40865	1.24%	0.137%
36	12.319	936	939	942	rVB3	18755	38656	1.17%	0.129%
37	12.376	942	944	946	rBV	73333	82641	2.51%	0.277%
38	12.411	946	947	950	rVB3	37586	68318	2.07%	0.229%
39	12.456	950	951	956	rBV	55959	50970	1.55%	0.171%
40	12.536	956	958	960	rBV	1399227	1191794	36.15%	3.990%
41	12.594	960	963	965	rBV3	23375	34882	1.06%	0.117%
42	12.685	967	971	975	rBV2	46981	91536	2.78%	0.306%
43	12.765	975	978	980	rBV	1156541	1289524	39.11%	4.317%
44	12.879	986	988	989	rBV	65365	65964	2.00%	0.221%
45	12.914	989	991	993	rVB	977603	1050542	31.86%	3.517%
46	12.982	993	997	998	rBV2	64662	81509	2.47%	0.273%
47	13.085	1001	1006	1008	rBV2	136977	234448	7.11%	0.785%
48	13.154	1010	1012	1014	rBV	152949	142966	4.34%	0.479%
49	13.188	1014	1015	1017	rBV	85488	94387	2.86%	0.316%
50	13.279	1022	1023	1025	rVB	48356	48235	1.46%	0.161%
51	13.314	1025	1026	1028	rBV	64043	64425	1.95%	0.216%
52	13.382	1031	1032	1034	rBV2	48124	64656	1.96%	0.216%
53	13.485	1039	1041	1045	rVV4	32076	71227	2.16%	0.238%
54	13.588	1048	1050	1053	rVB	66188	88628	2.69%	0.297%
55	13.702	1058	1060	1061	rBV	115181	142684	4.33%	0.478%
56	13.737	1061	1063	1064	rBV	55066	60348	1.83%	0.202%
57	13.954	1079	1082	1087	rVB2	1151615	2104002	63.82%	7.043%
58	14.057	1089	1091	1093	rVV	127318	115039	3.49%	0.385%
59	14.137	1096	1098	1099	rVV2	65073	71011	2.15%	0.238%
60	14.171	1099	1101	1103	rVB3	45118	68335	2.07%	0.229%
61	14.342	1114	1116	1117	rVB	70726	75679	2.30%	0.253%
62	14.377	1117	1119	1120	rVB2	42059	51475	1.56%	0.172%
63	14.434	1122	1124	1125	rBV2	71454	65142	1.98%	0.218%
64	14.960	1168	1170	1175	rBV	455896	932817	28.29%	3.123%
65	15.062	1177	1179	1182	rVB2	104711	125429	3.80%	0.420%
66	15.245	1193	1195	1198	rVB	300630	371149	11.26%	1.242%
67	15.302	1198	1200	1203	rBV	411561	496806	15.07%	1.663%
68	15.360	1203	1205	1207	rBV	464258	690936	20.96%	2.313%
69	15.817	1243	1245	1247	rBV2	35897	52898	1.60%	0.177%
70	16.023	1261	1263	1271	rVB2	57828	145626	4.42%	0.487%
71	16.720	1321	1324	1329	rVB2	155779	309232	9.38%	1.035%

LSC Area Percent Report

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Operator : UM/SJ
Sample : H3399-01 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-25

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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Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	16.891	1336	1339	1341	rBV	44244	69825	2.12%	0.234%
73	17.131	1356	1360	1365	rBV	115834	237055	7.19%	0.794%
74	17.337	1376	1378	1382	rVB	29962	54962	1.67%	0.184%

Sum of corrected areas: 29872955

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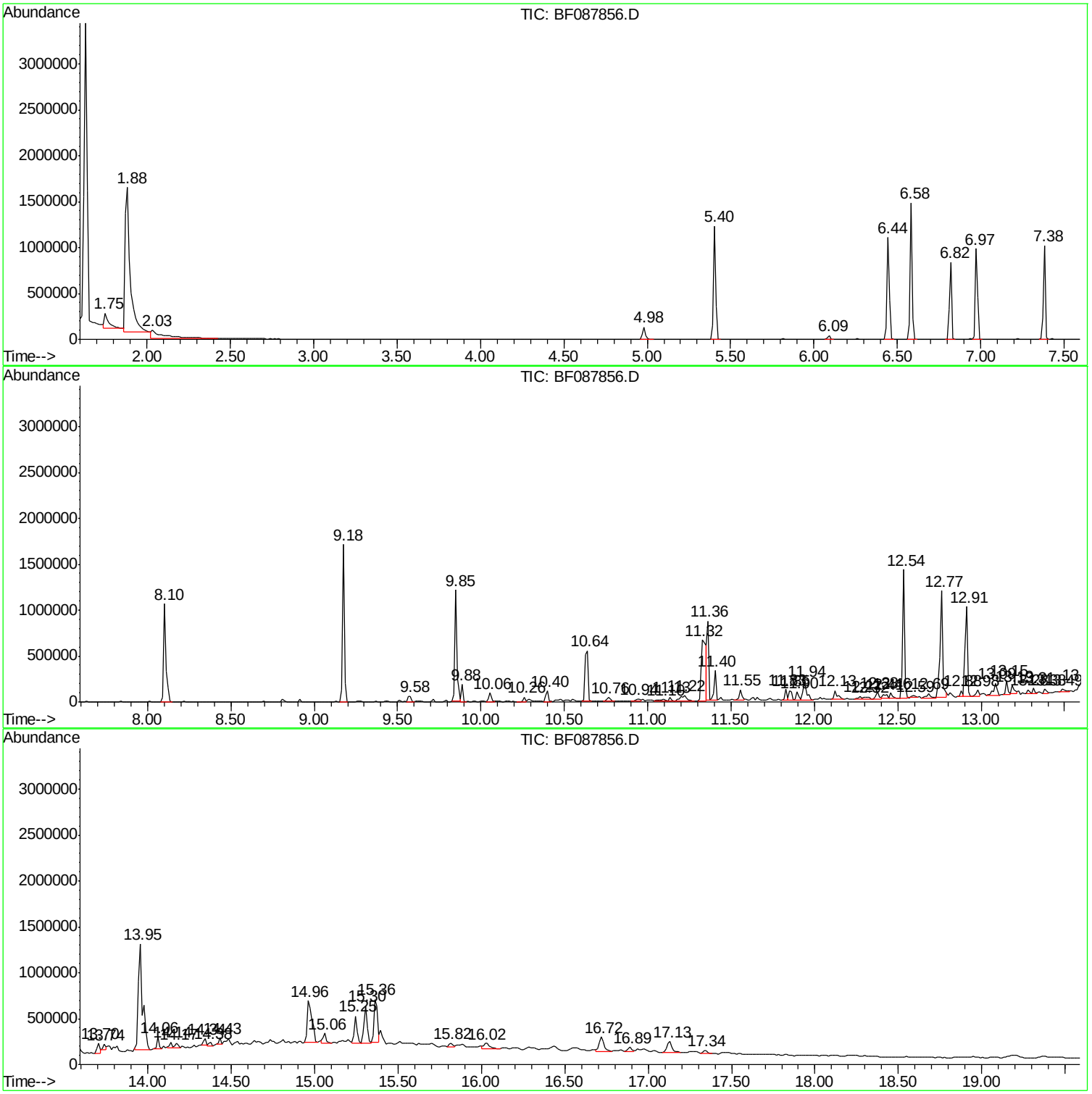
Instrument : BNA_F
ClientSampleId : SS-25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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\BF060916\
Data File : BF087856.D
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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

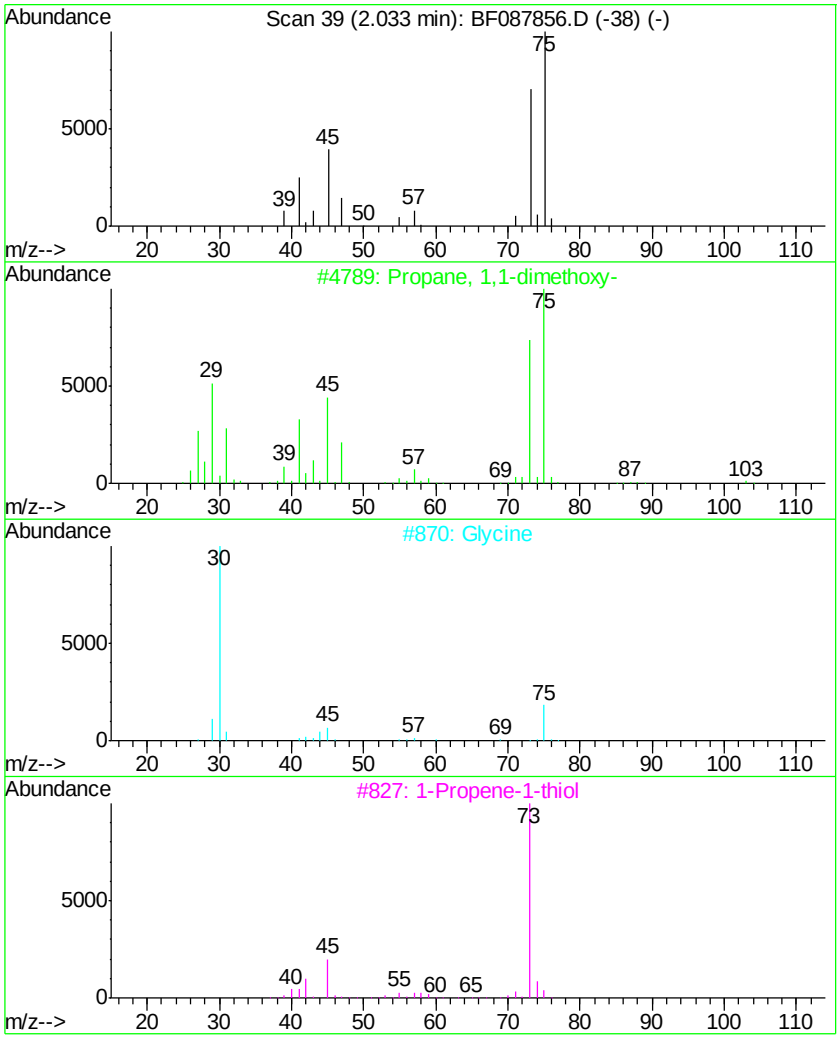
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

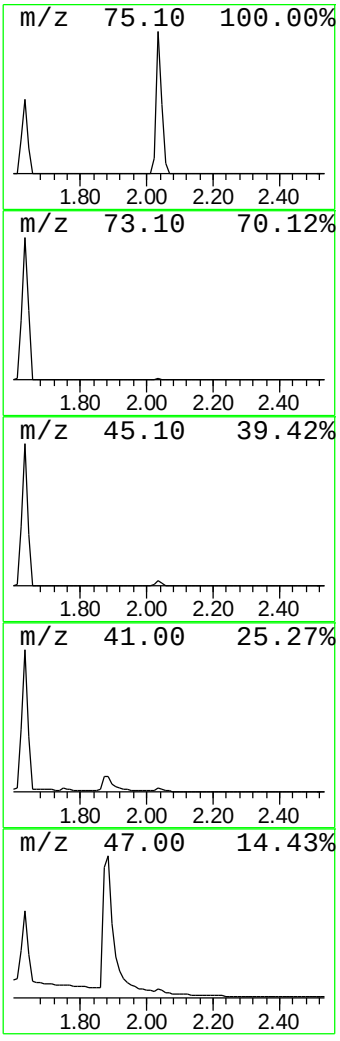
****

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.03	11.45 ng	462583	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2	Glycine	75	C2H5NO2	000056-40-6	7
3	1-Propene-1-thiol	74	C3H6S	000925-89-3	4
4	Silanol, trimethyl-	90	C3H10OSi	001066-40-6	4
5	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	4





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060916\
Data File : BF087856.D
Acq On : 9 Jun 2016 17:00
Operator : UM/SJ
Sample : H3399-01 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

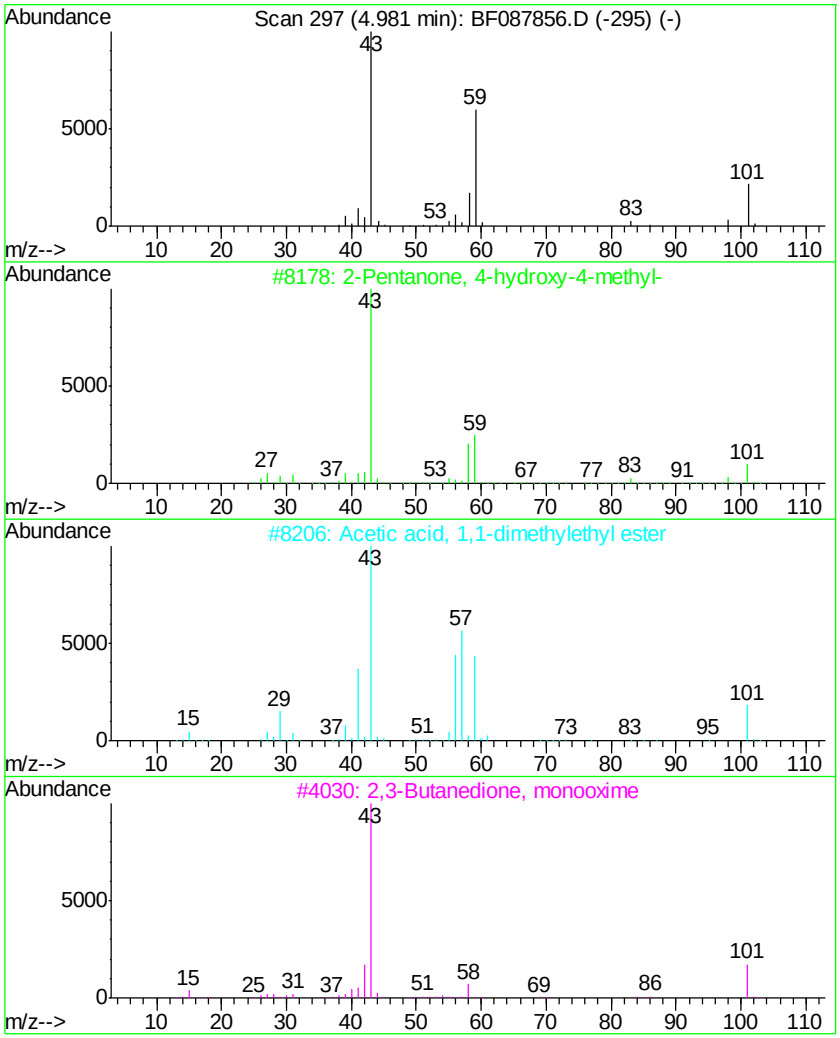
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

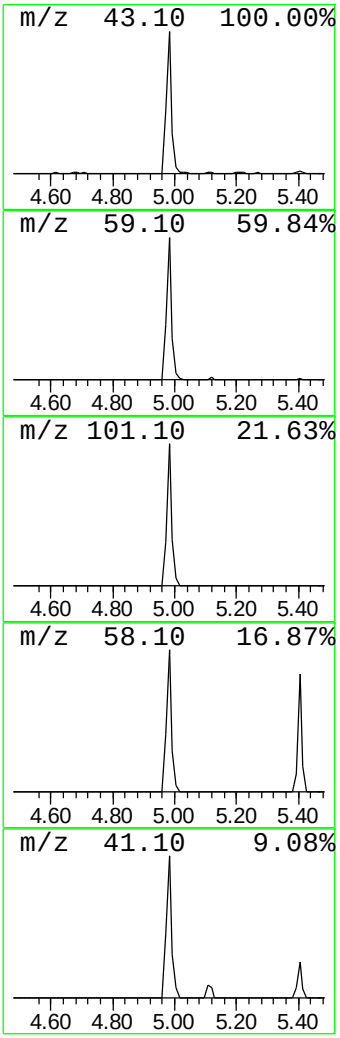
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	3.89 ng	156994	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Acetone	58	C3H6O	000067-64-1	9





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Operator : UM/SJ
Sample : H3399-01 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

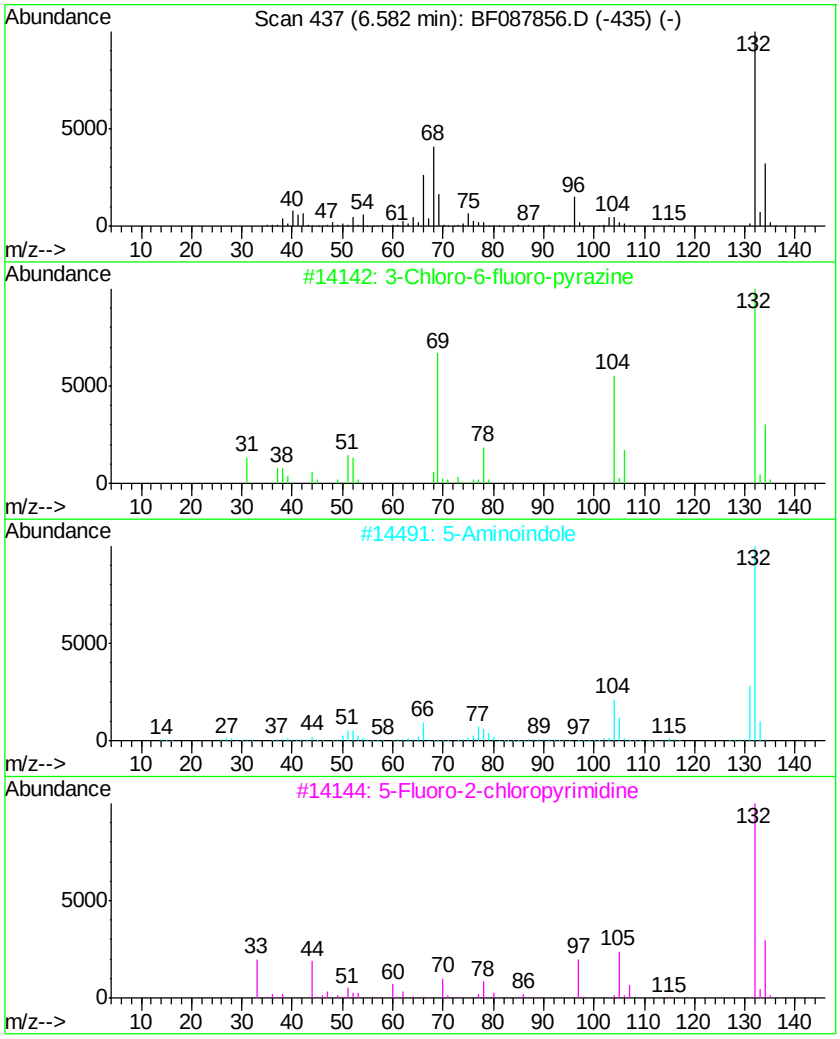
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

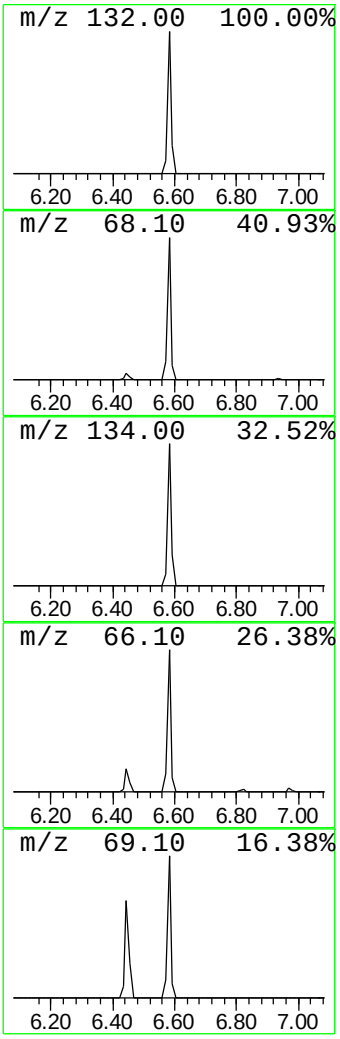
****

Peak Number 5 unknown6.58 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	31.79 ng	1284180	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060916\
Data File : BF087856.D
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Instrument : BNA_F
ClientSampleId : SS-25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

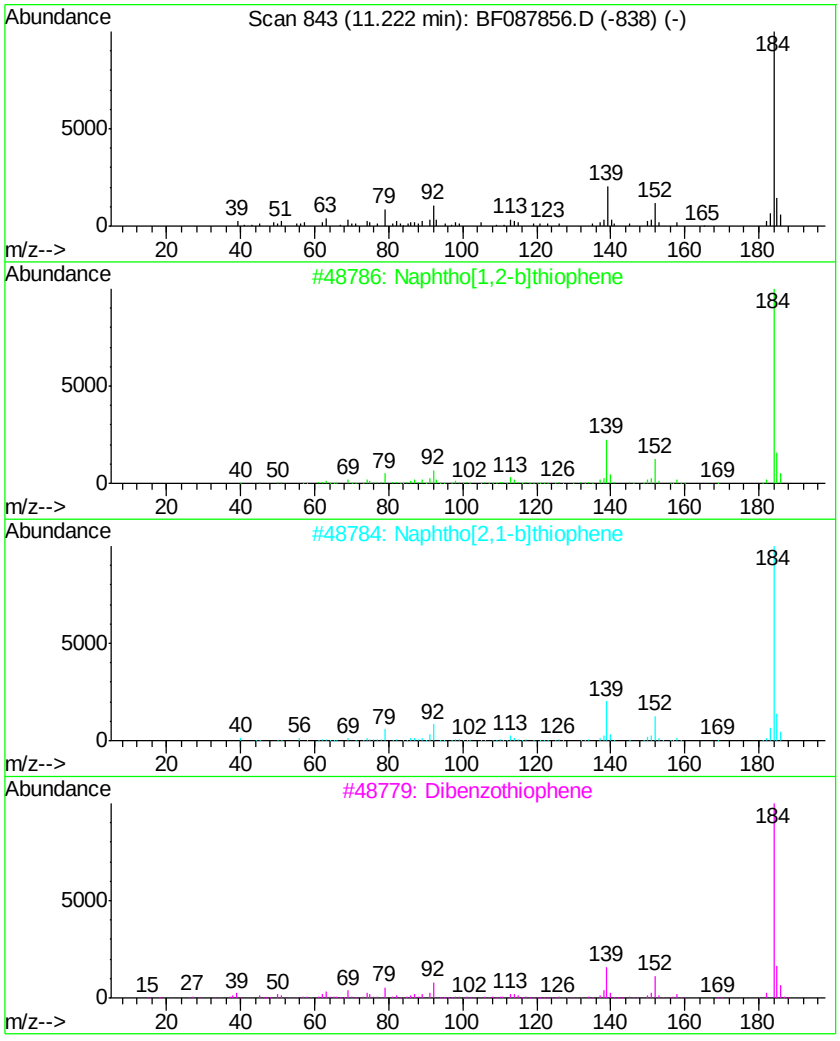
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

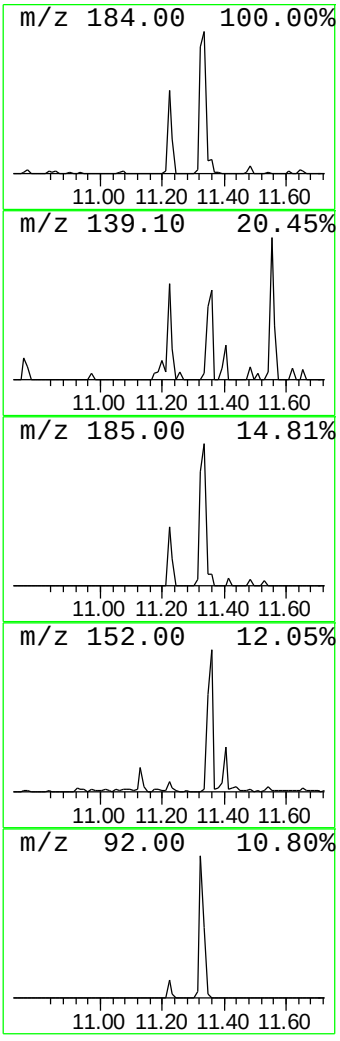
****

Peak Number 8 Naphtho[1,2-b]thiophene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.22	2.71 ng	178231	Phenanthrene-d10	11.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphtho[1,2-b]thiophene	184	C12H8S	000234-41-3	97
2	Naphtho[2,1-b]thiophene	184	C12H8S	000233-02-3	97
3	Dibenzothiophene	184	C12H8S	000132-65-0	97
4	Naphtho[2,3-b]thiophene	184	C12H8S	000268-77-9	95
5	Azuleno(2,1-b)thiophene	184	C12H8S	000248-13-5	94





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ALS Vial : 13 Sample Multiplier: 1

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

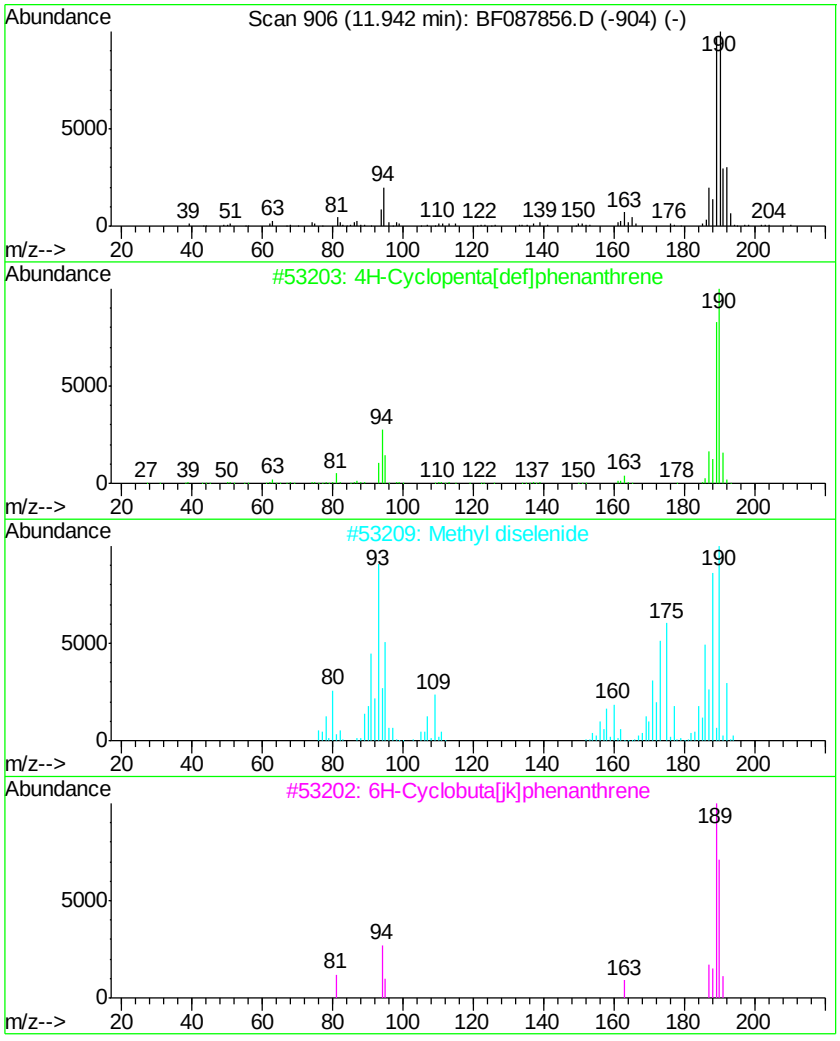
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

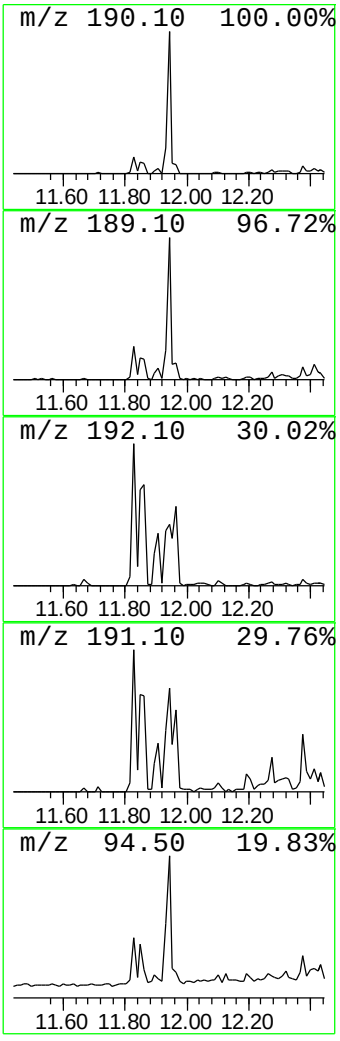
****

Peak Number 9 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	4.02 ng	263823	Phenanthrene-d10	11.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	94
2	Methyl diselenide	190	C2H6Se2	007101-31-7	55
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
4	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	47
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45





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Acq On : 9 Jun 2016 17:00
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Misc :
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Instrument : BNA_F
ClientSampleId : SS-25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

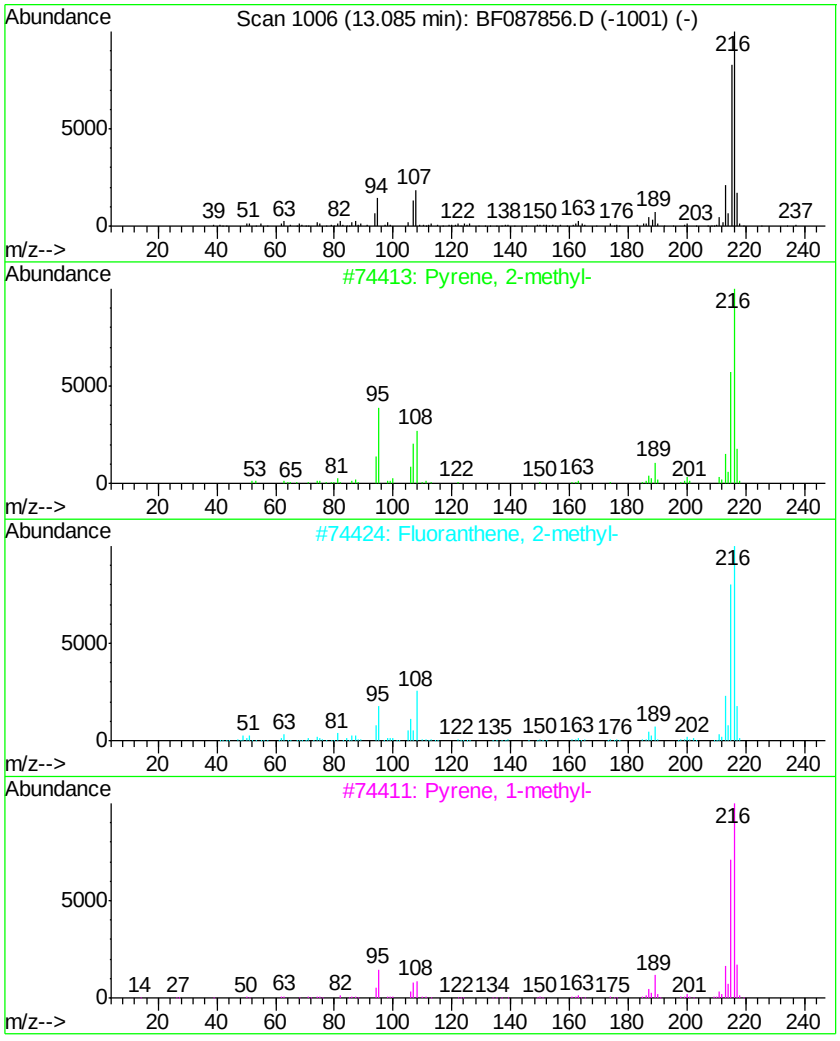
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

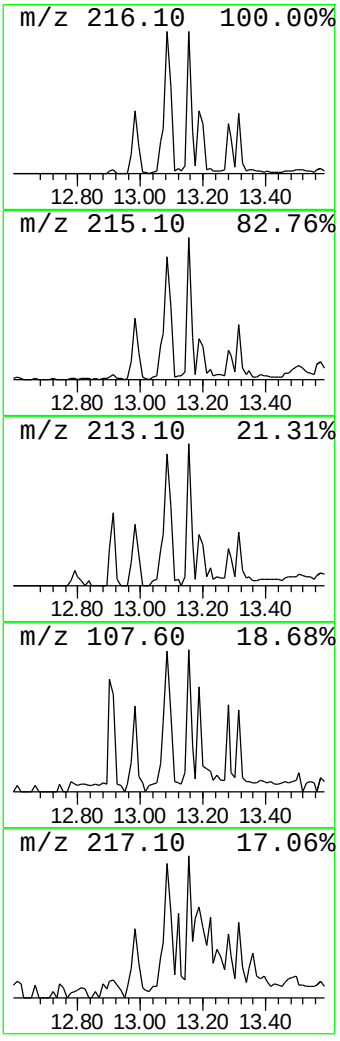
****

Peak Number 10 Pyrene, 2-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.09	2.23 ng	234448	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 2-methyl-	216	C17H12	003442-78-2	94
2	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	93
3	Pyrene, 1-methyl-	216	C17H12	002381-21-7	90
4	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
5	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060916\
Data File : BF087856.D
Acq On : 9 Jun 2016 17:00
Operator : UM/SJ
Sample : H3399-01 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

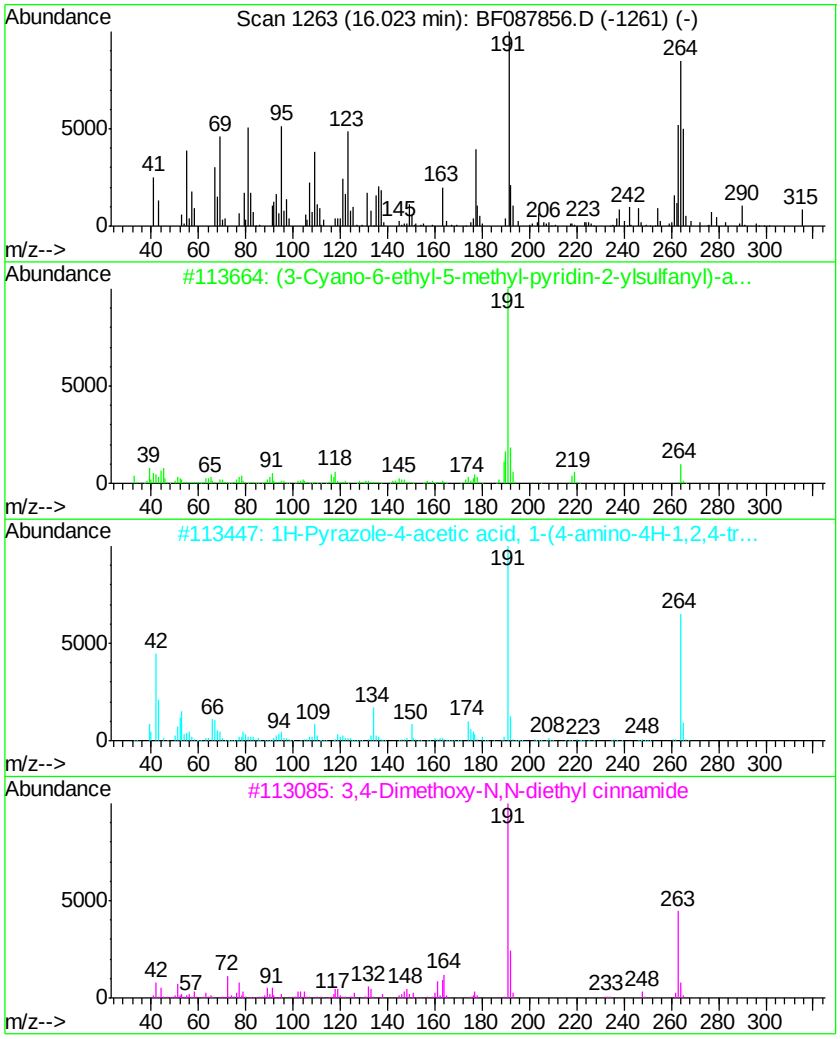
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

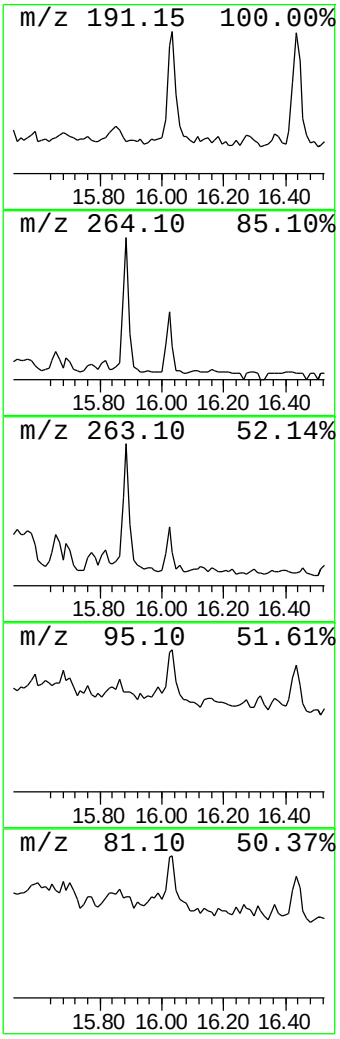
****

Peak Number 13 unknown16.02 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	4.22 ng	145626	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(3-Cyano-6-ethyl-5-methyl-pyridi...	264	C13H16N2O2S	1000300-45-4	35
2	1H-Pyrazole-4-acetic acid, 1-(4-...	264	C11H16N6O2	1000337-51-2	35
3	3,4-Dimethoxy-N,N-diethyl cinnamide	263	C15H21NO3	185410-48-4	22
4	Pyrido[3,4-d]pyridazin-1(2H)-one...	191	C8H9N5O	1000263-69-7	15
5	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	11





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060916\
Data File : BF087856.D
Acq On : 9 Jun 2016 17:00
Operator : UM/SJ
Sample : H3399-01 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

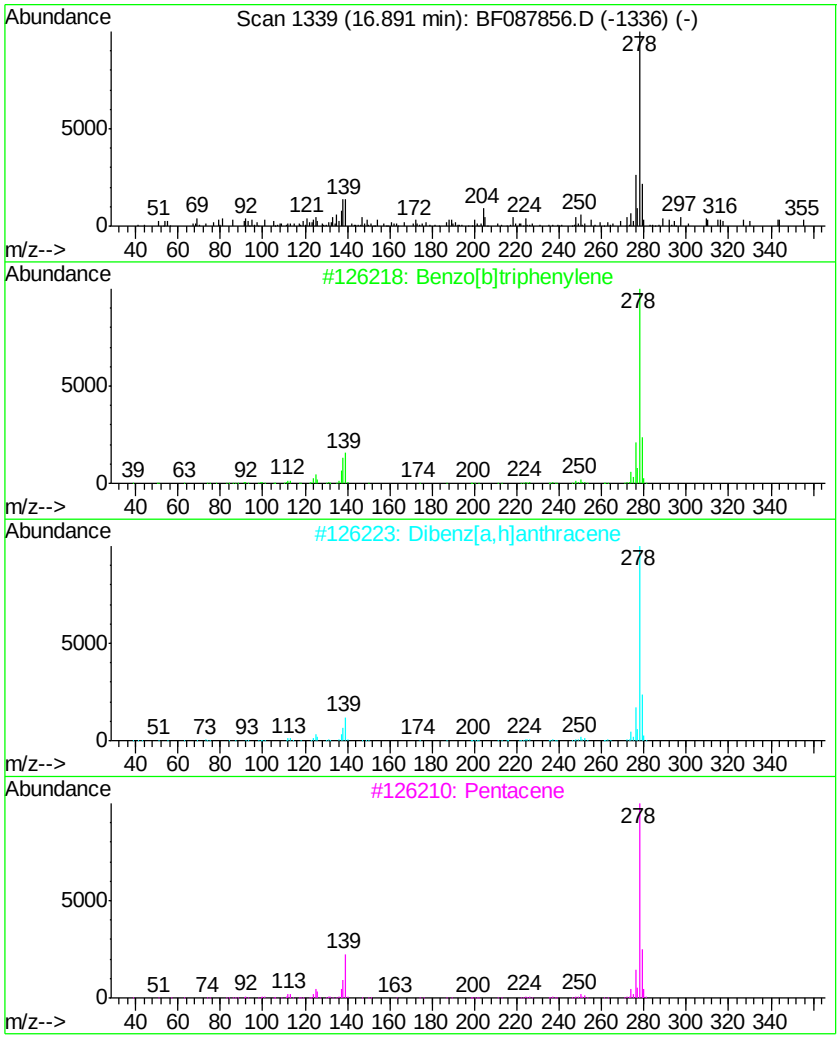
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

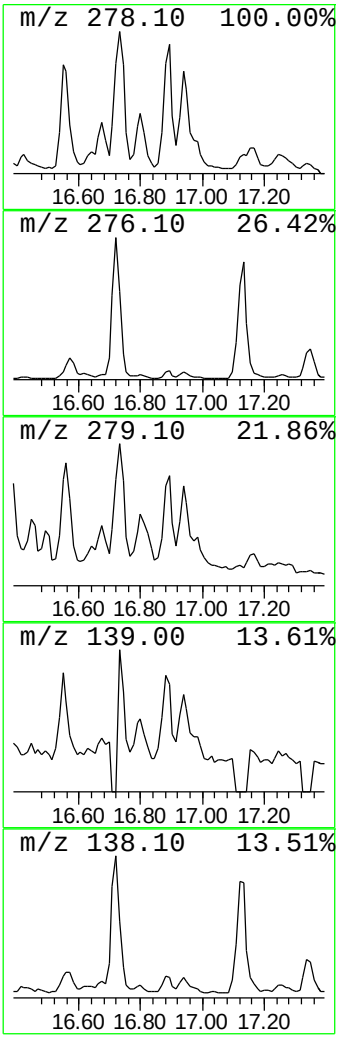
****

Peak Number 14 Benzo[b]triphenylene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.89	2.02 ng	69825	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]triphenylene	278	C22H14	000215-58-7	86
2	Dibenz[a,h]anthracene	278	C22H14	000053-70-3	86
3	Pentacene	278	C22H14	000135-48-8	86
4	Picene	278	C22H14	000213-46-7	86
5	Dibenz[a,j]anthracene	278	C22H14	000224-41-9	70





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060916\
Data File : BF087856.D
Acq On : 9 Jun 2016 17:00
Operator : UM/SJ
Sample : H3399-01 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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
Propane, 1,1-dime...	2.03	11.4	ng	462583	1	6.82	807938	20.0
2-Pentanone, 4-hy...	4.98	3.9	ng	156994	1	6.82	807938	20.0
unknown6.58	6.58	31.8	ng	1284180	1	6.82	807938	20.0
Naphtho[1,2-b]thi...	11.22	2.7	ng	178231	4	11.34	1313950	20.0
4H-Cyclopenta[def...	11.94	4.0	ng	263823	4	11.34	1313950	20.0
Pyrene, 2-methyl-	13.09	2.2	ng	234448	5	13.95	2104000	20.0
unknown16.02	16.02	4.2	ng	145626	6	15.36	690936	20.0
Benzo[b]triphenylene	16.89	2.0	ng	69825	6	15.36	690936	20.0