LSC Area Percent Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF101816\
Data File : BF090626.D
Acq On : 18 Oct 2016 11:42
Operator : UM/SJ
Sample : H5227-01 2X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1

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-BF101316.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	5.069	237	239	247	rBV	501297	637229	24.24%	1.701%
2	5.503	274	277	279	rBV	1753660	2455002	93.38%	6.552%
3	5.994	316	320	324	rBV	13076	31160	1.19%	0.083%
4	6.532	364	367	369	rBV	2053214	2533576	96.37%	6.762%
5	6.669	376	379	381	rBV	1891826	2629041	100.00%	7.017%
6	6.897	397	399	410	rBV	1374031	1338986	50.93%	3.574%
7	7.057	410	413	415	rBV	1480961	1780321	67.72%	4.752%
8	7.457	446	448	454	rBV	1496300	1556580	59.21%	4.154%
9	7.549	454	456	464	rVB	35599	88011	3.35%	0.235%
10	7.983	491	494	499	rVB6	14595	28907	1.10%	0.077%
11	8.189	509	512	514	rBV	1447393	1814904	69.03%	4.844%
12	8.818	565	567	571	rBV4	9724	26628	1.01%	0.071%
13	8.898	573	574	578	rVV	48415	46875	1.78%	0.125%
14	9.000	581	583	585	rBV	40798	44024	1.67%	0.117%
15	9.263	603	606	608	rBV	2599671	2254753	85.76%	6.018%
16	9.355	612	614	618	rVB3	35852	71916	2.74%	0.192%
17	9.526	627	629	631	rBV	18283	26807	1.02%	0.072%
18	9.595	633	635	637	rBV	33111	50482	1.92%	0.135%
19	9.652	639	640	643	rVV	495460	536208	20.40%	1.431%
20	9.721	643	646	651	rVB3	24699	54583	2.08%	0.146%
21	9.801	651	653	655	rBV	76353	76666	2.92%	0.205%
22	9.869	655	659	662	rVB2	38993	101842	3.87%	0.272%
23	9.938	663	665	667	rVV	1600458	1834935	69.79%	4.897%
24	9.972	667	668	671	rVB	175654	147660	5.62%	0.394%
25	10.098	677	679	681	rBV3	14535	26301	1.00%	0.070%
26	10.143	681	683	686	rVV	92516	124997	4.75%	0.334%
27	10.235	689	691	692	rVV2	19883	27102	1.03%	0.072%
28	10.269	692	694	697	rVB3	22280	48993	1.86%	0.131%
29	10.372	702	703	707	rVV2	78099	73130	2.78%	0.195%
30	10.441	707	709	711	rVV2	48569	59461	2.26%	0.159%
31	10.486	711	713	716	rVB	120083	127182	4.84%	0.339%
32	10.555	716	719	720	rBV	27966	31383	1.19%	0.084%
33	10.601	720	723	724	rVV2	40432	67165	2.55%	0.179%
34	10.646	725	727	729	rVV	39838	40217	1.53%	0.107%

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Misc :
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Instrument : BNA_F
ClientSampleId : 1

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 >
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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	10.726	732	734	737	rVV	1378654	1394972	53.06%	3.723%
36	10.806	740	741	743	rVV	44584	42661	1.62%	0.114%
37	10.852	743	745	749	rVB	98731	154019	5.86%	0.411%
38	10.932	749	752	755	rBV4	44159	65226	2.48%	0.174%
39	11.035	759	761	765	rBV5	28842	66070	2.51%	0.176%
40	11.298	780	784	785	rBV3	69365	88050	3.35%	0.235%
41	11.321	785	786	789	rVB	38845	56287	2.14%	0.150%
42	11.378	789	791	793	rBV	49888	57827	2.20%	0.154%
43	11.424	793	795	800	rBV2	1110520	2167435	82.44%	5.785%
44	11.504	801	802	808	rVB	188775	219325	8.34%	0.585%
45	11.652	813	815	820	rVV2	93410	168974	6.43%	0.451%
46	11.721	820	821	823	rVV2	41783	58348	2.22%	0.156%
47	11.778	824	826	828	rVV2	62370	62131	2.36%	0.166%
48	11.812	828	829	831	rVB	89192	74860	2.85%	0.200%
49	11.892	834	836	837	rBV2	23106	27326	1.04%	0.073%
50	11.926	837	839	840	rVV	55412	60335	2.29%	0.161%
51	11.961	840	842	843	rVV	114505	125731	4.78%	0.336%
52	12.041	847	849	854	rVB2	147663	220963	8.40%	0.590%
53	12.224	863	865	871	rBV4	42969	94847	3.61%	0.253%
54	12.406	880	881	885	rBV3	24594	42089	1.60%	0.112%
55	12.475	885	887	889	rBV	69893	101810	3.87%	0.272%
56	12.521	889	891	893	rVB	45668	56831	2.16%	0.152%
57	12.567	893	895	897	rBV2	34401	48348	1.84%	0.129%
58	12.635	899	901	904	rBV	479678	688536	26.19%	1.838%
59	12.681	904	905	909	rVB4	16160	35058	1.33%	0.094%
60	12.795	913	915	918	rBV3	20174	33227	1.26%	0.089%
61	12.875	918	922	925	rBV	520944	872906	33.20%	2.330%
62	13.012	932	934	938	rVB	1296199	1307966	49.75%	3.491%
63	13.092	938	941	945	rVB3	53661	95842	3.65%	0.256%
64	13.195	947	950	952	rBV2	105805	169517	6.45%	0.452%
65	13.264	954	956	958	rBV2	77451	80491	3.06%	0.215%
66	13.298	958	959	962	rVV	64114	87346	3.32%	0.233%
67	13.389	965	967	969	rVB	35439	44286	1.68%	0.118%
68	13.424	969	970	972	rBV	52499	50823	1.93%	0.136%
69	13.709	993	995	997	rVB	44100	49616	1.89%	0.132%
70	13.915	1011	1013	1018	rVB4	138768	212879	8.10%	0.568%
71	14.075	1023	1027	1033	rBV2	1125241	2159355	82.13%	5.763%

LSC Area Percent Report

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Data File : BF090626.D
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Sample : H5227-01 2X
Misc :
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Instrument : BNA_F
ClientSampleId : 1

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-BF101316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	14.178	1034	1036	1038	rVB	78602	84678	3.22%	0.226%
73	15.104	1115	1117	1122	rBV	463071	1044599	39.73%	2.788%
74	15.401	1141	1143	1147	rVB	239636	371834	14.14%	0.992%
75	15.470	1147	1149	1152	rVV	424095	593323	22.57%	1.584%
76	15.538	1152	1155	1165	rVB2	875650	1845186	70.18%	4.925%
77	15.675	1165	1167	1172	rBV4	62968	120017	4.57%	0.320%
78	16.224	1213	1215	1222	rVB2	111285	265363	10.09%	0.708%
79	16.658	1251	1253	1260	rVB2	105785	219740	8.36%	0.586%
80	16.978	1277	1281	1286	rVB2	175811	414039	15.75%	1.105%
81	17.413	1315	1319	1327	rBV	151269	373617	14.21%	0.997%

Sum of corrected areas: 37467736

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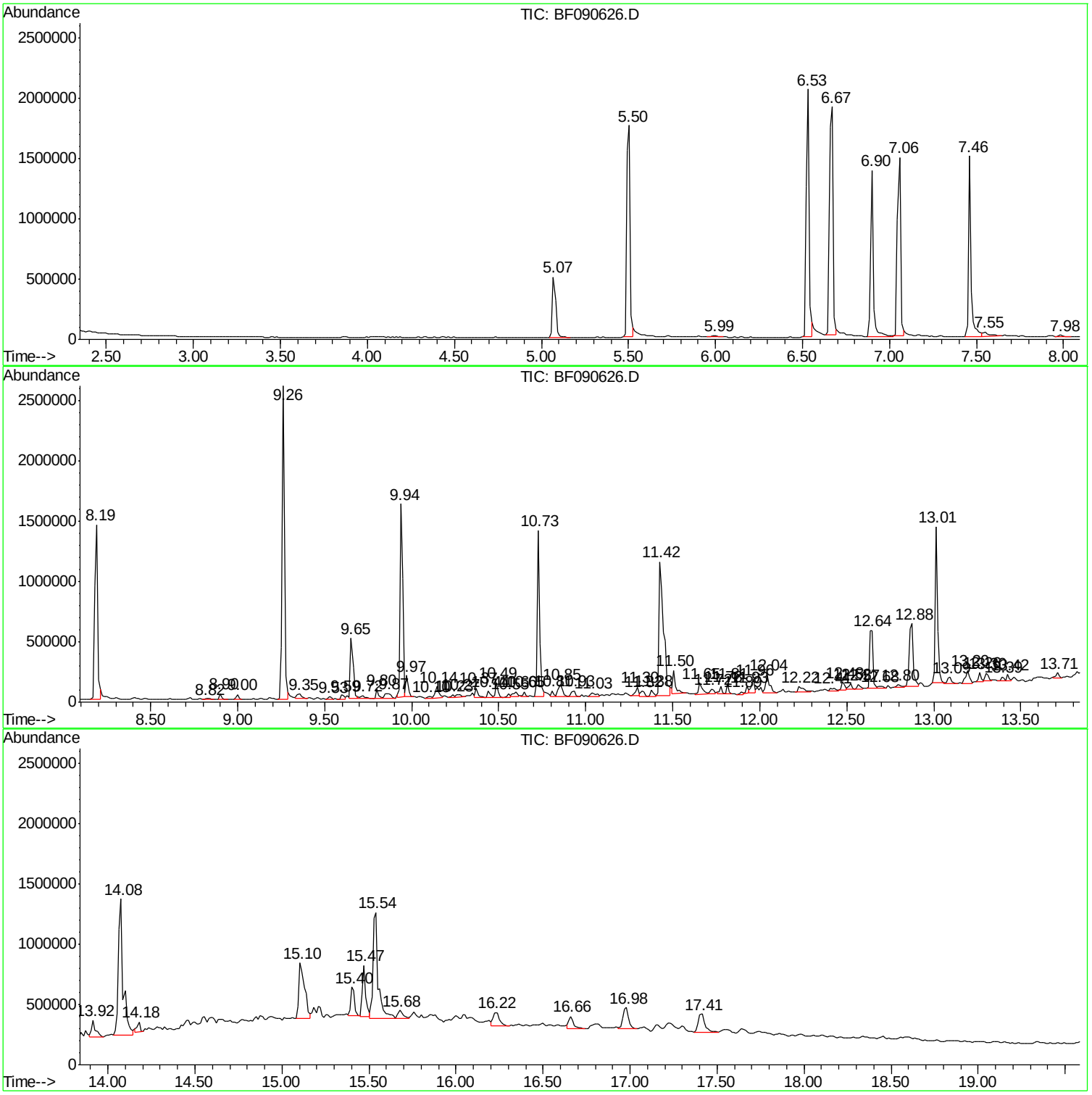
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.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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Acq On : 18 Oct 2016 11:42
Operator : UM/SJ
Sample : H5227-01 2X
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Instrument : BNA_F
ClientSampleId : 1

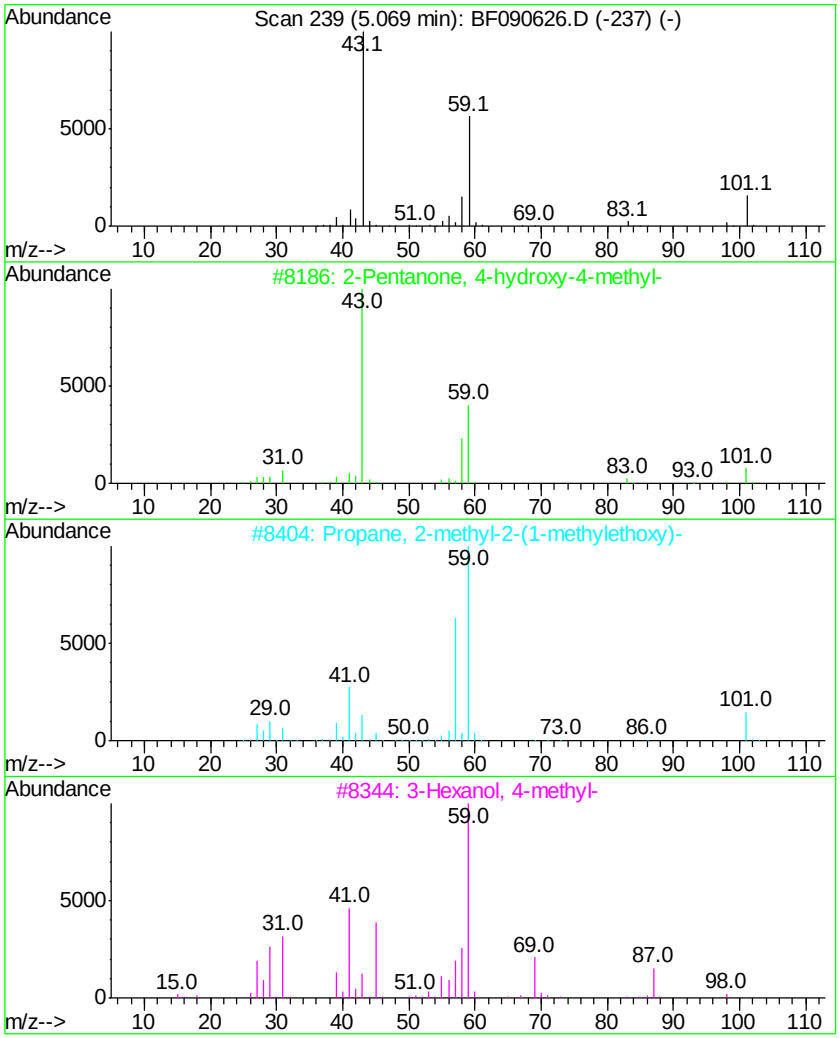
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

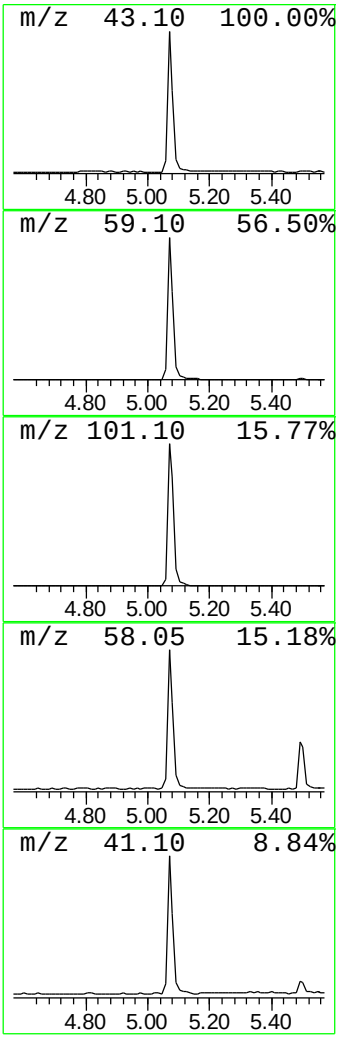
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	9.52 ng	637229	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
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





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TIC Library : C:\DATABASE\NIST11.L
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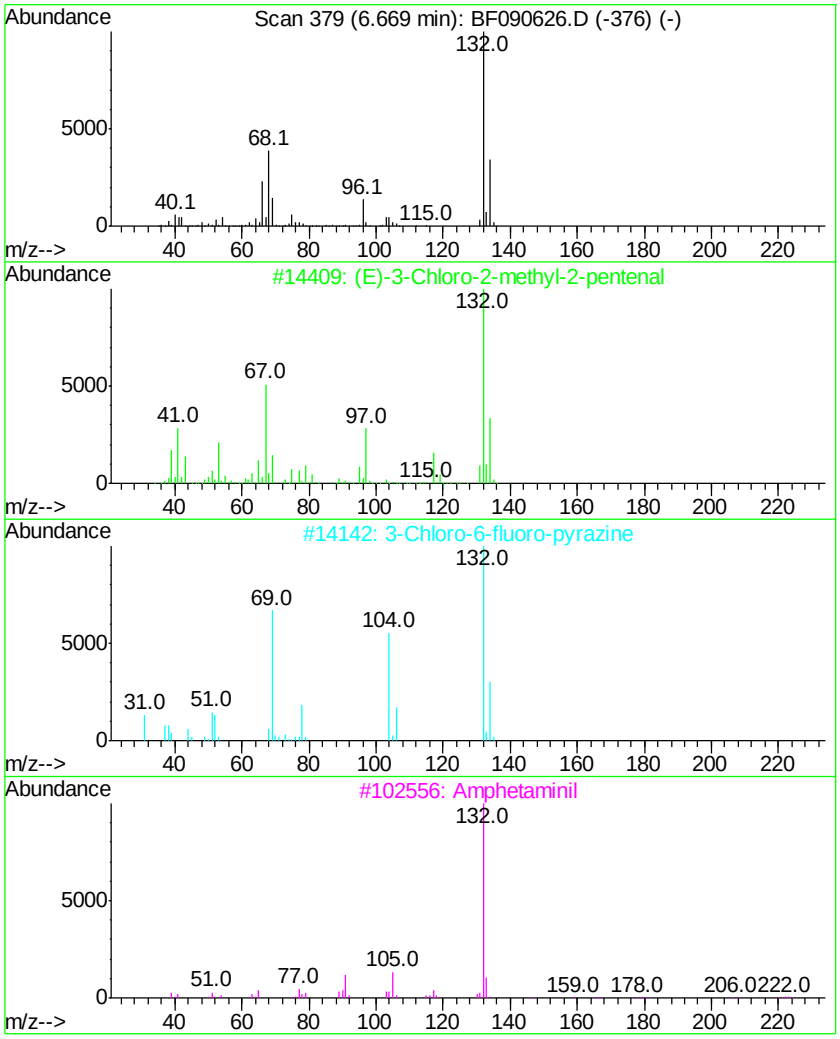
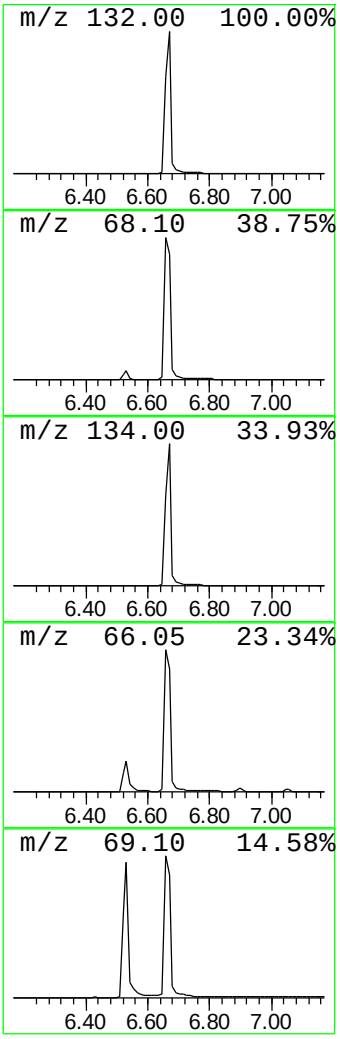
****

Peak Number 2 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	39.27 ng	2629040	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	Amphetaminil	250	C17H18N2	017590-01-1	10
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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TIC Library : C:\DATABASE\NIST11.L
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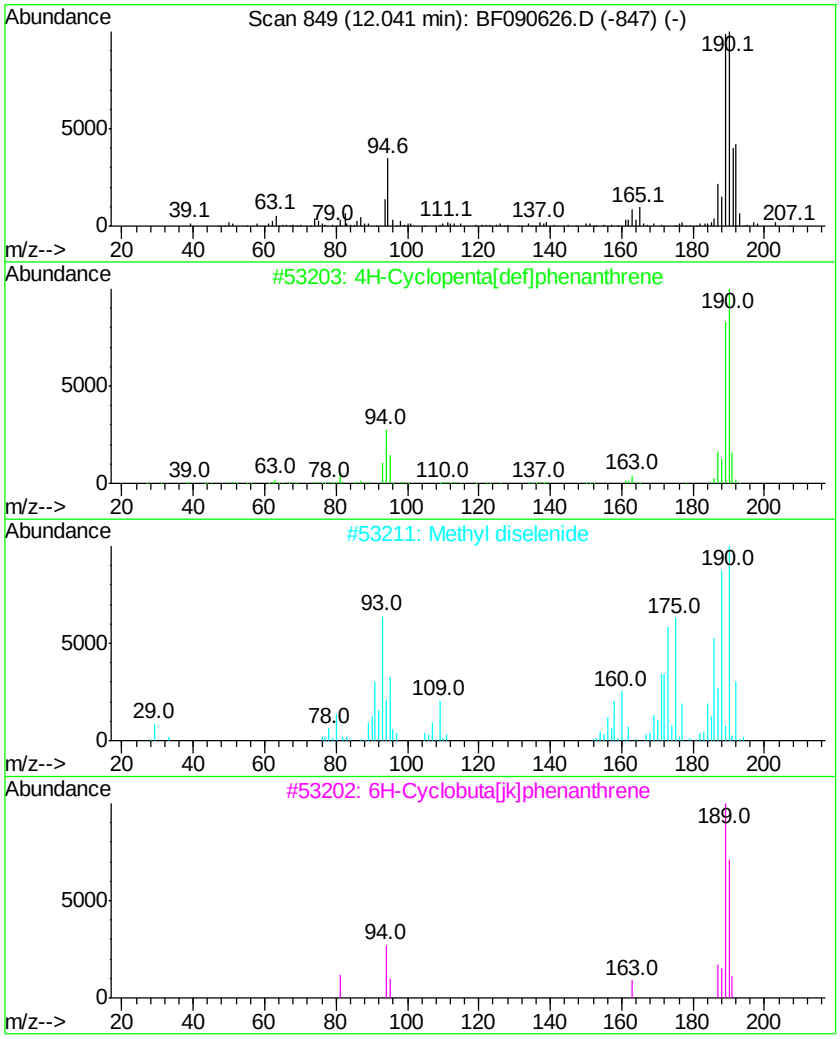
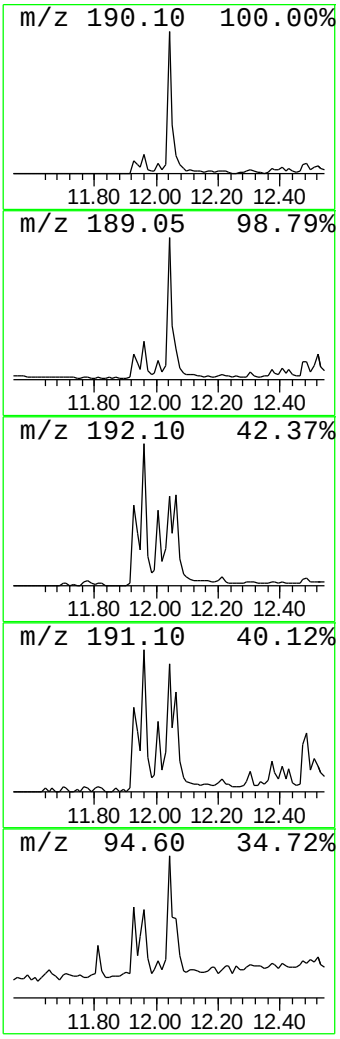
****

Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.04	2.04 ng	220963	Phenanthrene-d10	11.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	Methyl diselenide	190	C2H6Se2	007101-31-7	43
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	42
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	37
5	Megastigmatrienone	190	C13H18O	038818-55-2	18





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Instrument : BNA_F
ClientSampleId : 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

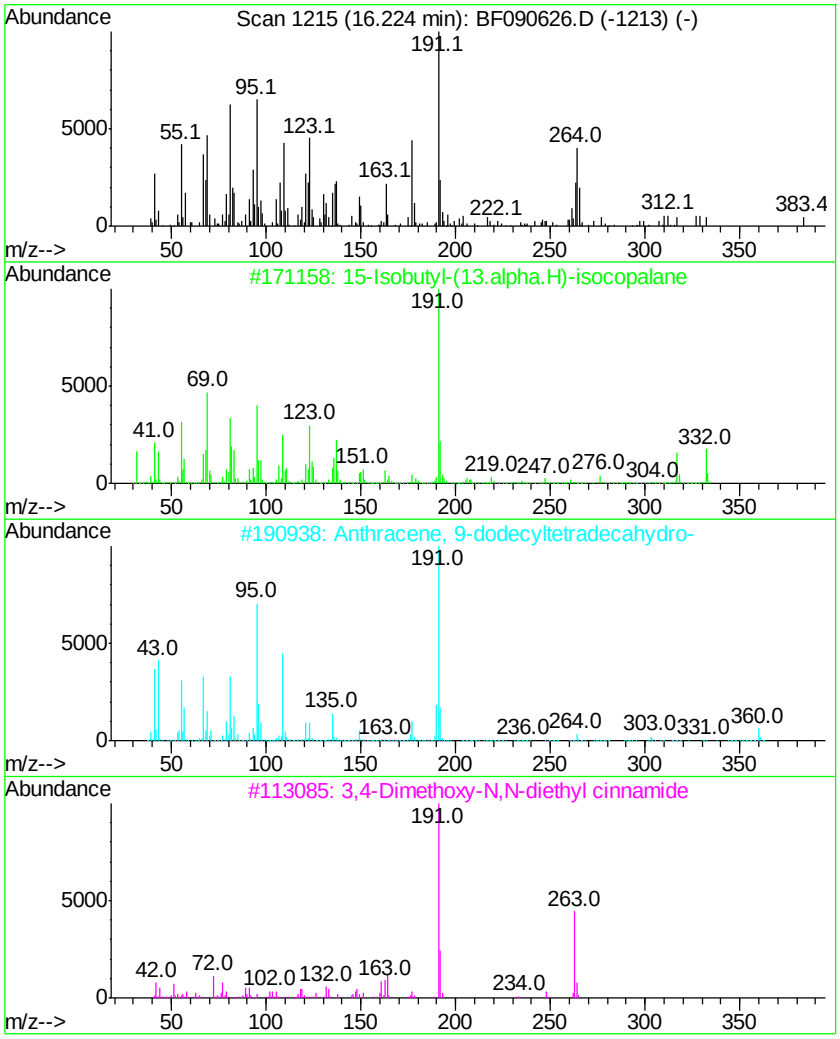
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

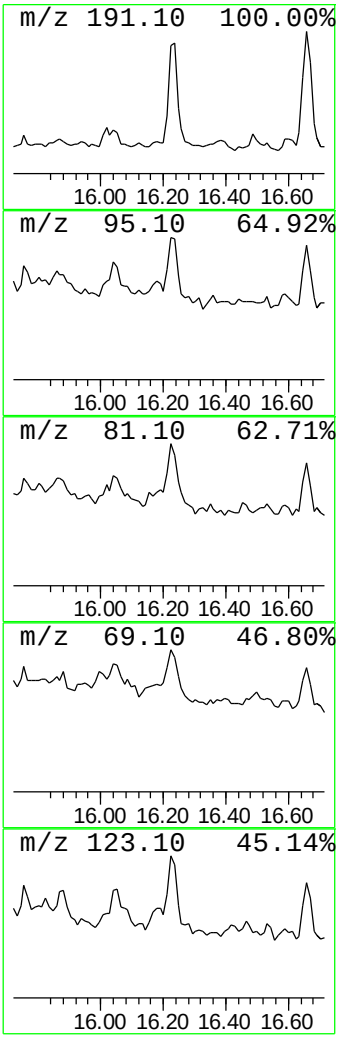
****

Peak Number 6 15-Isobutyl-(13.alpha.H)-is... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.22	2.88 ng	265363	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	15-Isobutyl-(13.alpha.H)-isocopa...	332	C24H44	087953-47-7	53
2	Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	38
3	3,4-Dimethoxy-N,N-diethyl cinnamide	263	C15H21NO3	185410-48-4	22
4	Anthracene, 9-cyclohexyltetradec...	274	C20H34	055255-70-4	22
5	Urea, N-(4,5-dihydro-5-methyl-2-...	329	C17H16FN3OS	1000350-96-1	14





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

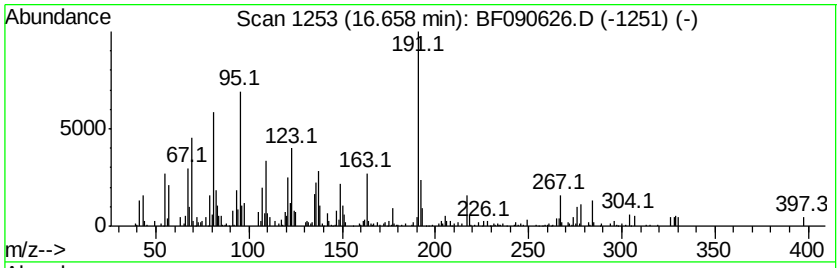
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

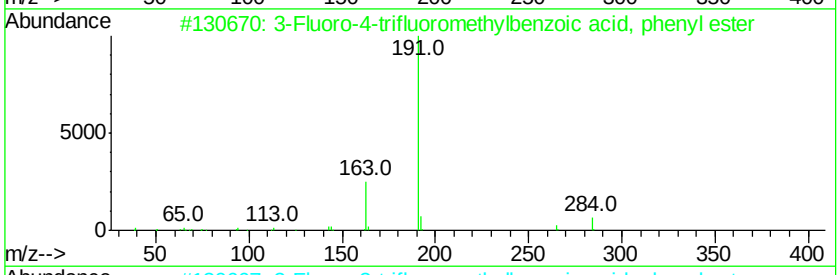
****

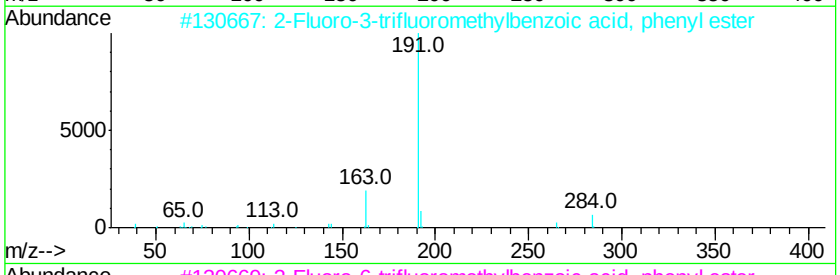
Peak Number 7 unknown16.66 Concentration Rank 6

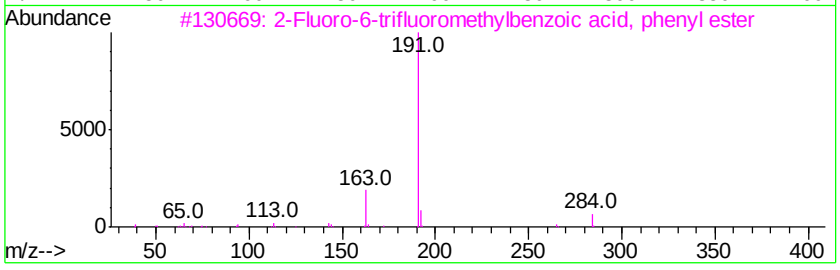
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.66	2.38 ng	219740	Perylene-d12	15.54

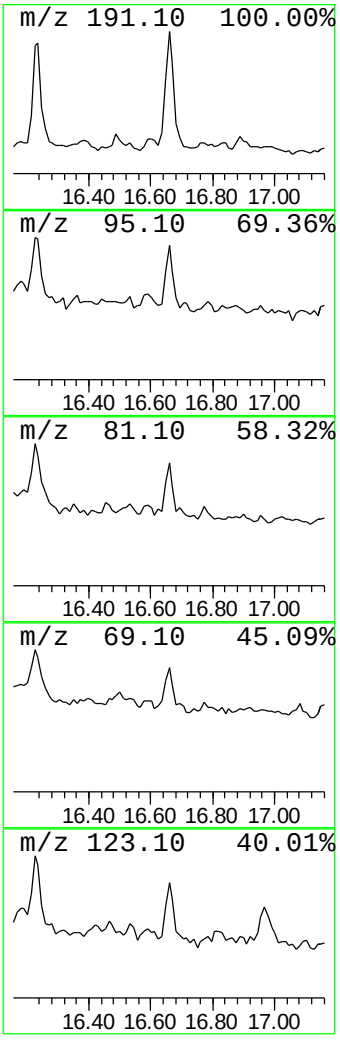
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Fluoro-4-trifluoromethylbenzoi...	284	C14H8F4O2	1000357-93-7	30
2	2-Fluoro-3-trifluoromethylbenzoi...	284	C14H8F4O2	1000357-64-3	30
3	2-Fluoro-6-trifluoromethylbenzoi...	284	C14H8F4O2	1000357-69-4	30
4	3-Fluoro-5-trifluoromethylbenzoi...	284	C14H8F4O2	1000357-95-5	30
5	5-Fluoro-2-trifluoromethylbenzoi...	284	C14H8F4O2	1000357-62-7	27











Tentatively Identified Compound (LSC) summary

Data Path : U:\HPCHEM1\BNA_F\DATA\BF101816\
Data File : BF090626.D
Acq On : 18 Oct 2016 11:42
Operator : UM/SJ
Sample : H5227-01 2X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.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
2-Pentanone, 4-hy...	5.07	9.5	ng	637229	1	6.90	1338990	20.0
unknown6.67	6.67	39.3	ng	2629040	1	6.90	1338990	20.0
4H-Cyclopenta[def...	12.04	2.0	ng	220963	4	11.42	2167440	20.0
15-Isobutyl-(13.a...	16.22	2.9	ng	265363	6	15.54	1845190	20.0
unknown16.66	16.66	2.4	ng	219740	6	15.54	1845190	20.0