LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF013016\
Data File : BF084691.D
Acq On : 30 Jan 2016 17:36
Operator : SJ/IZ
Sample : H1261-09 5X
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SCARBOROUGH1516-00(0-4)

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-BF012916.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	4.178	180	183	187	rBV	88570	118087	8.28%	0.591%
2	4.876	241	244	246	rBV	1022580	1351707	94.83%	6.764%
3	5.310	280	282	285	rBV	746153	1040683	73.01%	5.208%
4	5.721	316	318	321	rVB	105862	91293	6.40%	0.457%
5	5.984	338	341	343	rVB2	8714	15609	1.10%	0.078%
6	6.247	360	364	368	rVB4	7642	18892	1.33%	0.095%
7	6.373	372	375	377	rBV	900136	1041112	73.04%	5.210%
8	6.487	383	385	388	rBV	1110501	1071464	75.17%	5.362%
9	6.727	404	406	408	rBV	1064494	1140237	79.99%	5.706%
10	6.876	417	419	422	rVB	985593	862433	60.50%	4.316%
11	7.287	453	455	457	rBV	863867	692827	48.60%	3.467%
12	8.007	516	518	521	rBV	1512405	1425445	100.00%	7.133%
13	8.442	554	556	558	rBV	15530	17000	1.19%	0.085%
14	9.093	610	613	615	rBV	967761	1153338	80.91%	5.772%
15	9.173	617	620	622	rVV3	10330	15464	1.08%	0.077%
16	9.425	641	642	645	rVB3	15449	16587	1.16%	0.083%
17	9.493	645	648	650	rBV	83183	119354	8.37%	0.597%
18	9.619	658	659	661	rVB	23425	23060	1.62%	0.115%
19	9.710	665	667	669	rBV	18704	22964	1.61%	0.115%
20	9.768	669	672	674	rBV	1046921	1423072	99.83%	7.121%
21	9.962	688	689	691	rBV	17267	14930	1.05%	0.075%
22	10.008	691	693	696	rVB3	15606	22491	1.58%	0.113%
23	10.076	696	699	701	rBV4	9547	17127	1.20%	0.086%
24	10.202	709	710	712	rVB	41682	35883	2.52%	0.180%
25	10.419	727	729	732	rBV	16253	28924	2.03%	0.145%
26	10.476	732	734	738	rVB3	9768	21665	1.52%	0.108%
27	10.545	738	740	743	rBV	633844	571321	40.08%	2.859%
28	10.671	749	751	755	rBV2	36710	65253	4.58%	0.327%
29	10.876	764	769	770	rBV3	9219	21424	1.50%	0.107%
30	11.116	789	790	796	rVB2	24861	53979	3.79%	0.270%
31	11.242	798	801	803	rVV	1488223	1302230	91.36%	6.517%
32	11.311	804	807	809	rVB2	31048	40974	2.87%	0.205%
33	11.425	814	817	819	rVV2	13160	19134	1.34%	0.096%
34	11.482	819	822	823	rVV3	10064	19100	1.34%	0.096%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
ClientSampleId : SCARBOROUGH1516-00(0-4)

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-BF012916.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.551	826	828	829	rVV	20090	22630	1.59%	0.113%
36	11.573	829	830	834	rVB2	16150	20416	1.43%	0.102%
37	11.745	843	845	846	rBV	35933	38071	2.67%	0.191%
38	11.768	846	847	850	rVV	54174	52217	3.66%	0.261%
39	11.848	852	854	860	rVV	44070	75021	5.26%	0.375%
40	11.951	860	863	867	rVV3	15507	45160	3.17%	0.226%
41	12.042	868	871	875	rVV5	17135	41265	2.89%	0.206%
42	12.191	881	884	885	rBV3	11321	19484	1.37%	0.098%
43	12.294	890	893	894	rVV	41183	44732	3.14%	0.224%
44	12.328	894	896	899	rVB2	15280	37361	2.62%	0.187%
45	12.374	899	900	902	rVB	32066	31762	2.23%	0.159%
46	12.454	904	907	909	rBV	105750	149516	10.49%	0.748%
47	12.499	909	911	914	rBV3	13342	22882	1.61%	0.115%
48	12.671	923	926	928	rBV2	170342	230581	16.18%	1.154%
49	12.739	930	932	934	rVB2	24290	26146	1.83%	0.131%
50	12.796	935	937	938	rBV	17072	26395	1.85%	0.132%
51	12.819	938	939	942	rVB	597521	715383	50.19%	3.580%
52	12.899	943	946	950	rBV3	26784	55193	3.87%	0.276%
53	13.002	952	955	957	rVB	30562	53605	3.76%	0.268%
54	13.071	957	961	962	rBV2	33158	46625	3.27%	0.233%
55	13.105	962	964	968	rBV	37578	38015	2.67%	0.190%
56	13.197	971	972	974	rBV	35218	39435	2.77%	0.197%
57	13.231	974	975	977	rVB	23967	20208	1.42%	0.101%
58	13.368	984	987	988	rBV	45852	52885	3.71%	0.265%
59	13.414	988	991	994	rVB4	29499	53460	3.75%	0.268%
60	13.517	998	1000	1003	rVB2	20124	40608	2.85%	0.203%
61	13.619	1006	1009	1011	rBV	38124	70276	4.93%	0.352%
62	13.734	1016	1019	1022	rBV3	72504	144142	10.11%	0.721%
63	13.802	1022	1025	1027	rVV3	27701	78331	5.50%	0.392%
64	13.871	1028	1031	1038	rVB	1214584	1347731	94.55%	6.744%
65	14.259	1063	1065	1066	rVB	39583	40017	2.81%	0.200%
66	14.294	1066	1068	1070	rBV	30859	33160	2.33%	0.166%
67	14.385	1072	1076	1081	rVV4	34902	142612	10.00%	0.714%
68	14.877	1116	1119	1123	rVB	119145	231408	16.23%	1.158%
69	14.957	1124	1126	1128	rBV3	65564	105733	7.42%	0.529%
70	15.140	1140	1142	1145	rVB	71923	101008	7.09%	0.505%
71	15.197	1145	1147	1150	rVB	96543	124048	8.70%	0.621%

LSC Area Percent Report

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Data File : BF084691.D
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Operator : SJ/IZ
Sample : H1261-09 5X
Misc :
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Instrument : BNA_F
ClientSampleId : SCARBOROUGH1516-00(0-4)

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-BF012916.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	15.265	1150	1153	1155	rBV	723048	1120047	78.58%	5.605%
73	15.688	1188	1190	1193	rBV	108827	162151	11.38%	0.811%
74	16.568	1264	1267	1271	rBV2	50577	128618	9.02%	0.644%
75	16.957	1299	1301	1304	rBV	34252	66764	4.68%	0.334%
76	18.408	1424	1428	1433	rVB4	68878	192906	13.53%	0.965%

Sum of corrected areas: 19983071

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF013016\
Data File : BF084691.D
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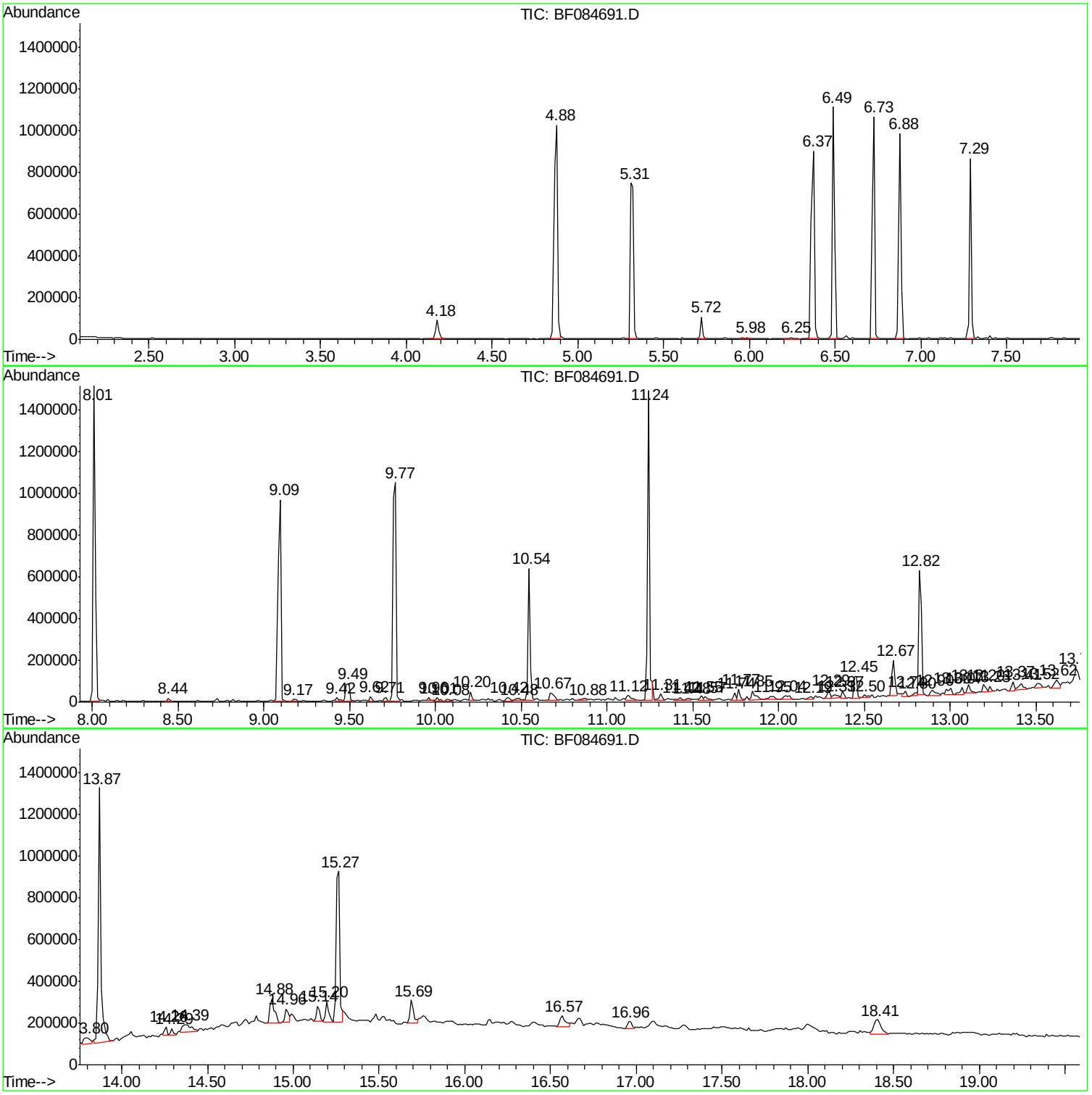
Sample : H1261-09 5X
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SCARBOROUGH1516-00(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.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\BF013016\
Data File : BF084691.D
Acq On : 30 Jan 2016 17:36
Operator : SJ/IZ
Sample : H1261-09 5X
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Instrument :
BNA_F
ClientSampleId :
SCARBOROUGH1516-00(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

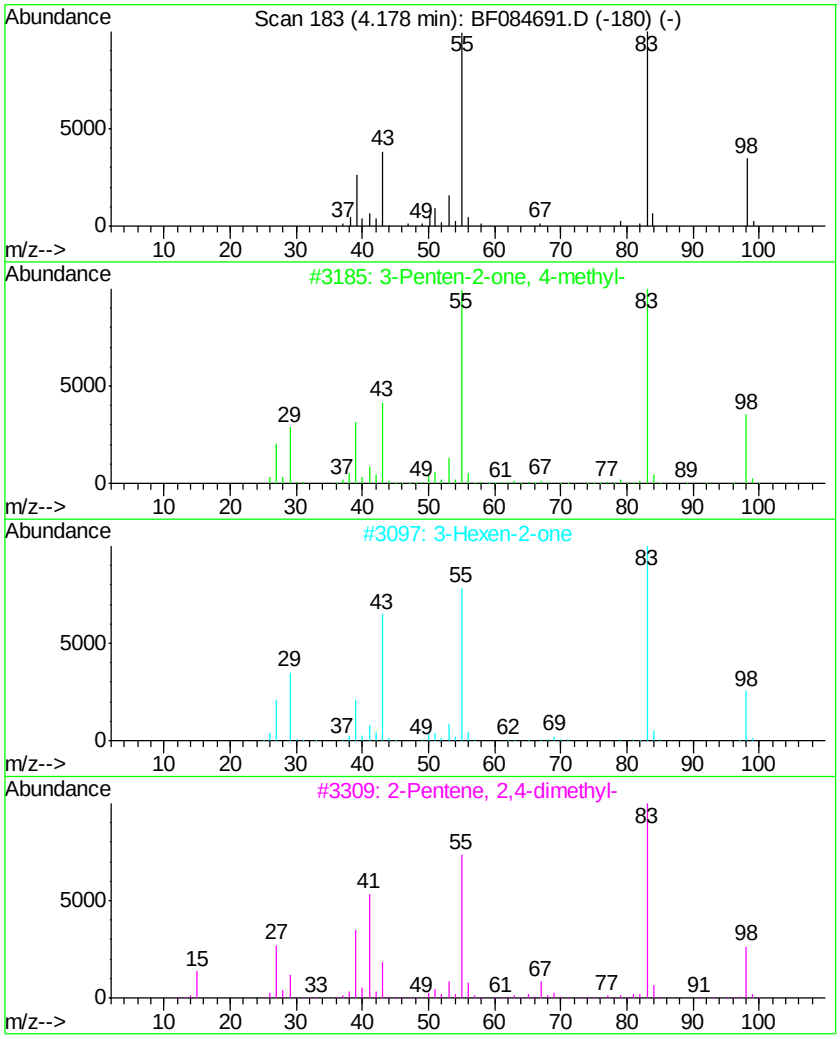
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

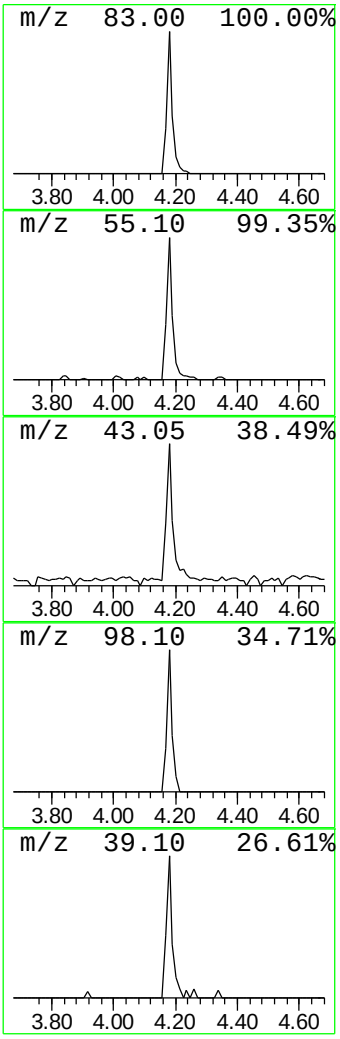
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.18	2.07 ng	118087	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2	3-Hexen-2-one	98	C6H10O	000763-93-9	90
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF013016\
Data File : BF084691.D
Acq On : 30 Jan 2016 17:36
Operator : SJ/IZ
Sample : H1261-09 5X
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SCARBOROUGH1516-00(0-4)

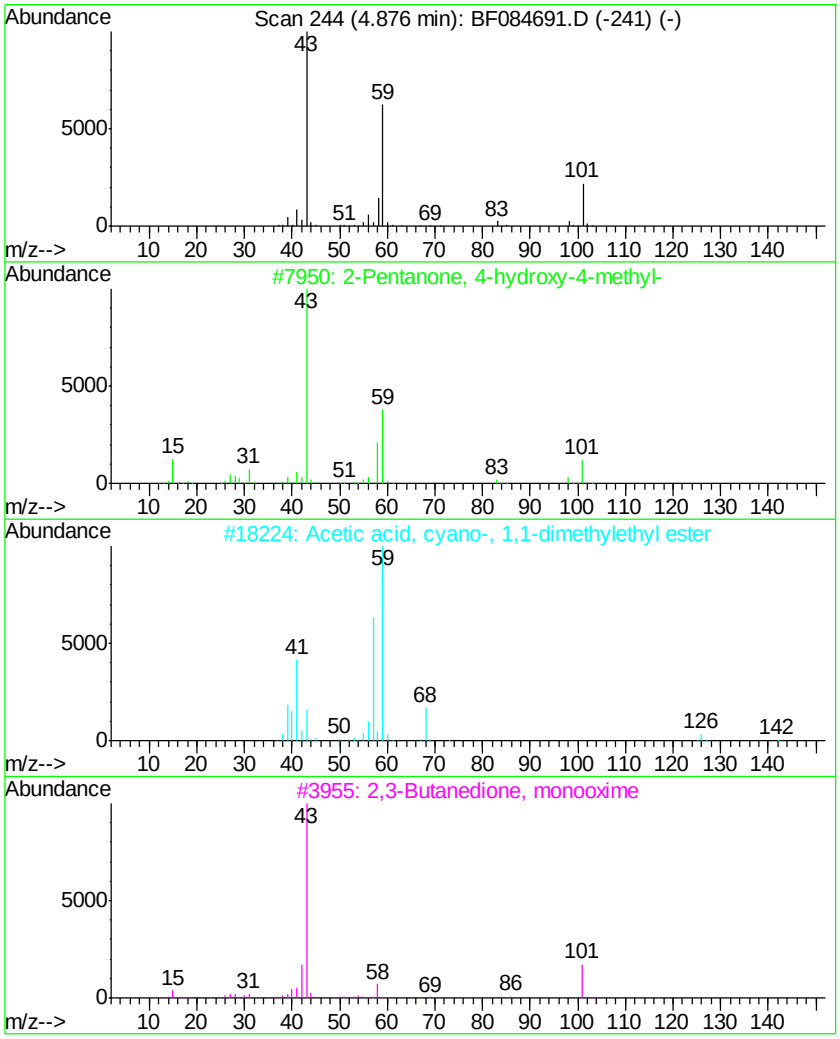
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

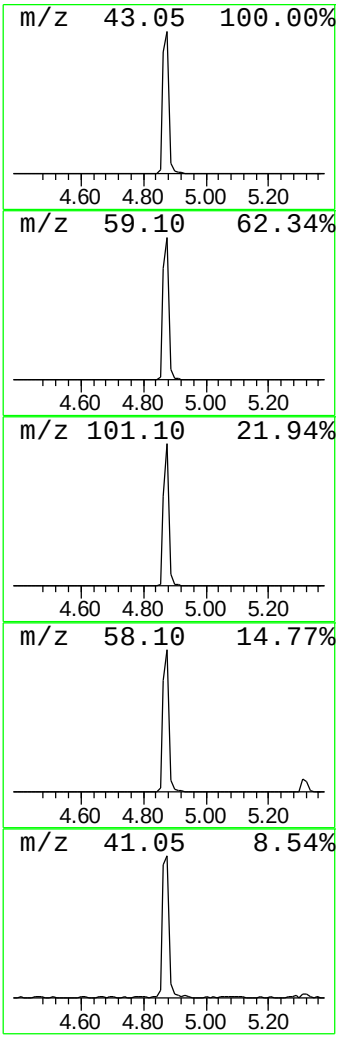
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	23.71 ng	1351710	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Guanidine	59	CH5N3	000113-00-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Operator : SJ/IZ
Sample : H1261-09 5X
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SCARBOROUGH1516-00(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

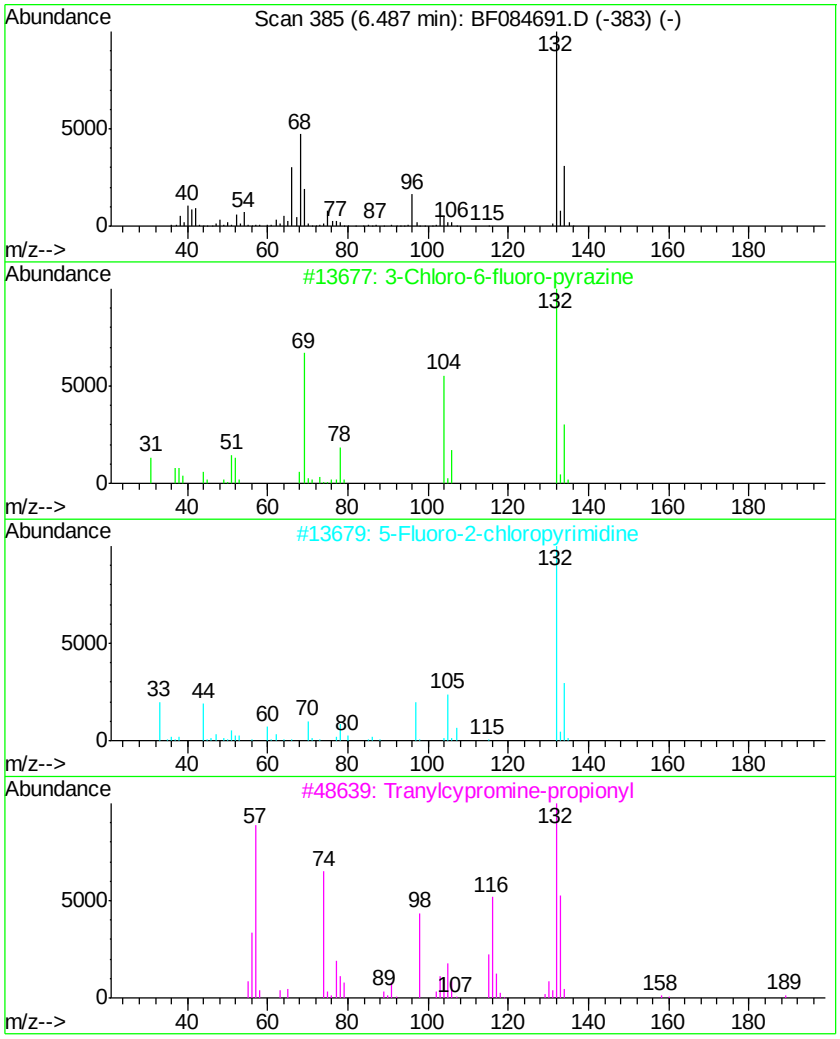
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

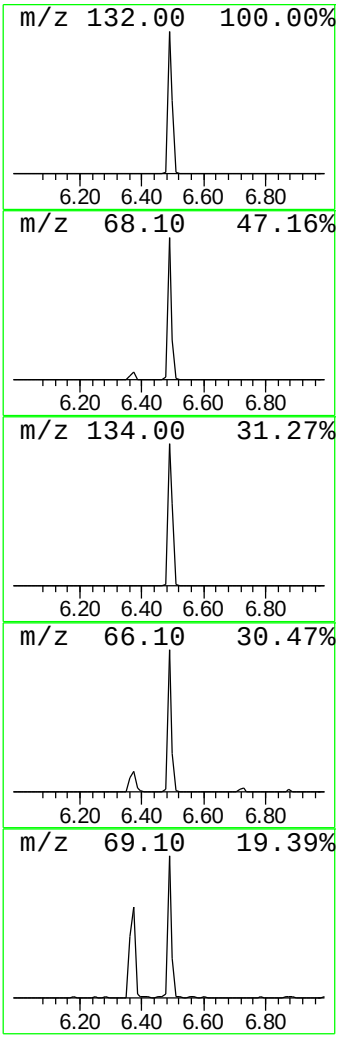
****

Peak Number 3 unknown6.49 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	18.79 ng	1071460	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





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BNA_F
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SCARBOROUGH1516-00(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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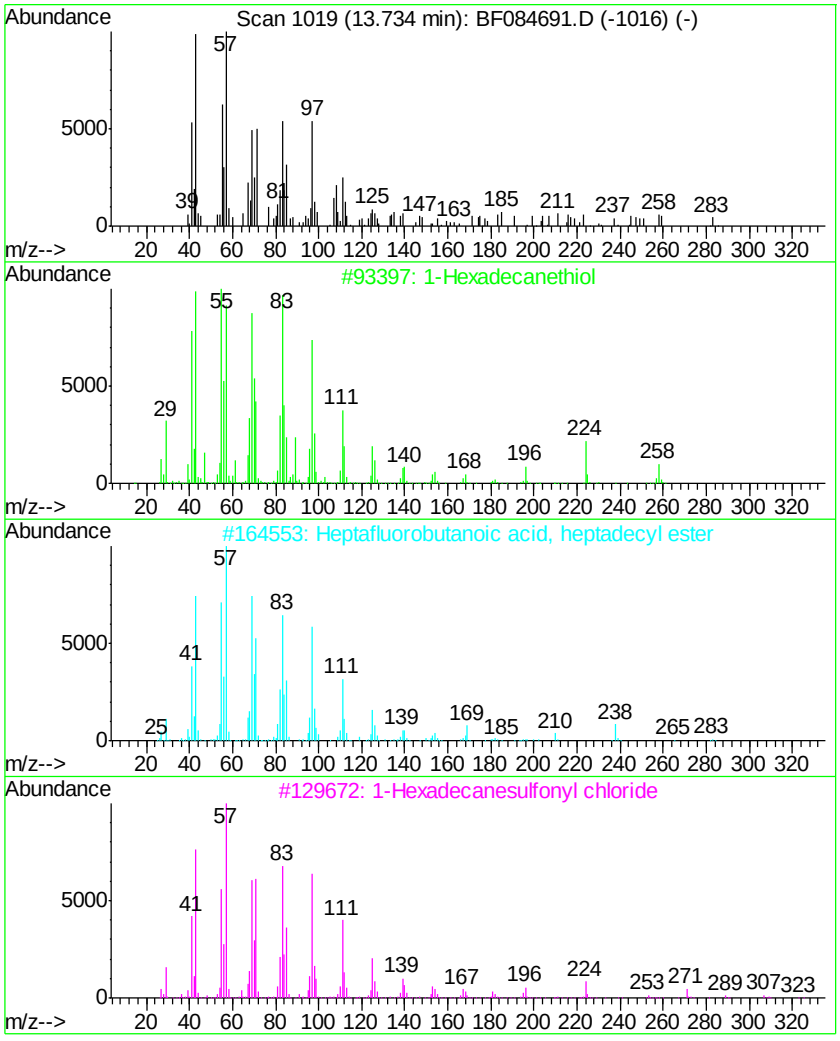
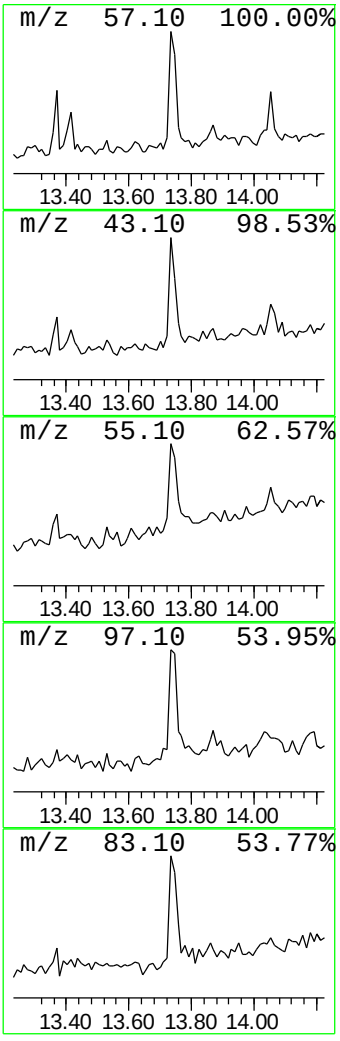
Peak Number 5 1-Hexadecanethiol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	2.14 ng	144142	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanethiol	258	C16H34S	002917-26-2	95
2	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	81
3	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	74
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	74
5	1-Docosene	308	C22H44	001599-67-3	68





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

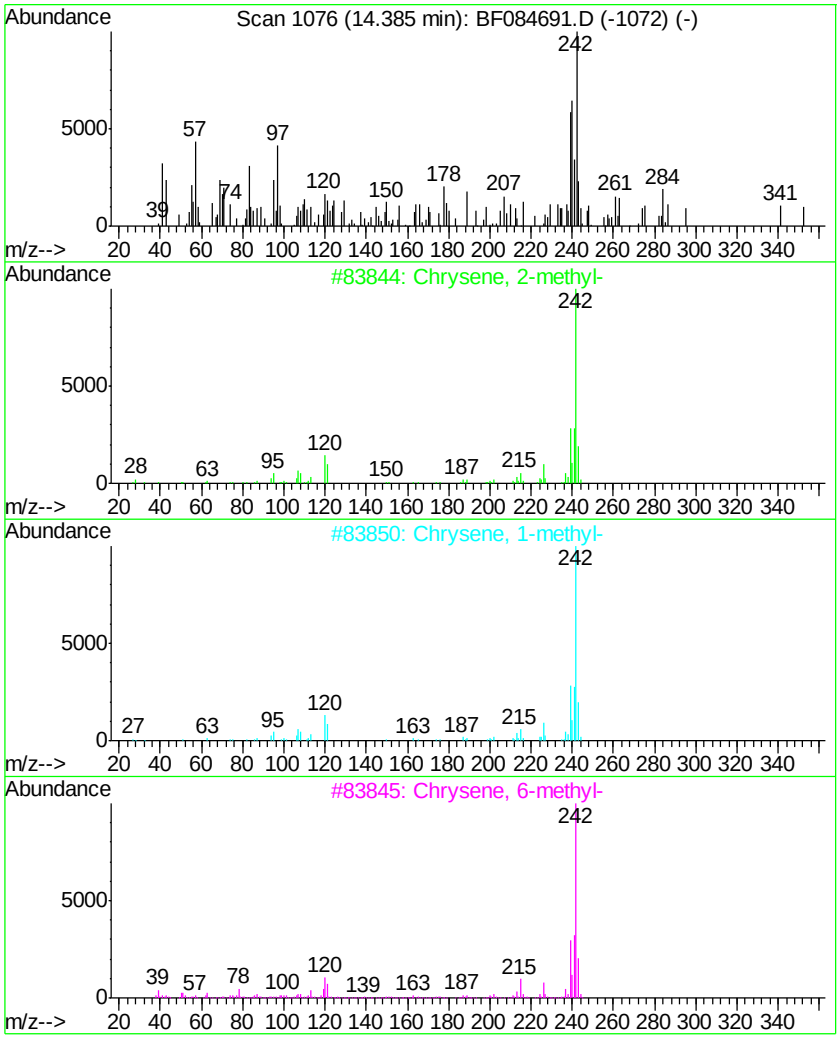
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

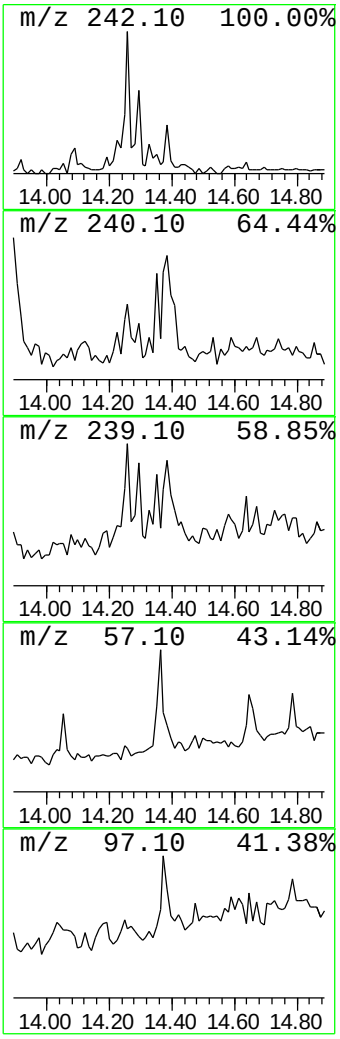
****

Peak Number 6 unknown14.39 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.39	2.12 ng	142612	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Chrysene, 2-methyl-	242	C19H14	003351-32-4	38
2	Chrysene, 1-methyl-	242	C19H14	003351-28-8	30
3	Chrysene, 6-methyl-	242	C19H14	003697-24-3	25
4	Benzonitrile, 2-(2-chlorobenzyli...	240	C14H9ClN2	104830-19-5	22
5	4b,10b-Dihydro-4b,10b-methanochr...	242	C19H14	071949-03-6	22





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Operator : SJ/IZ
Sample : H1261-09 5X
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SCARBOROUGH1516-00(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

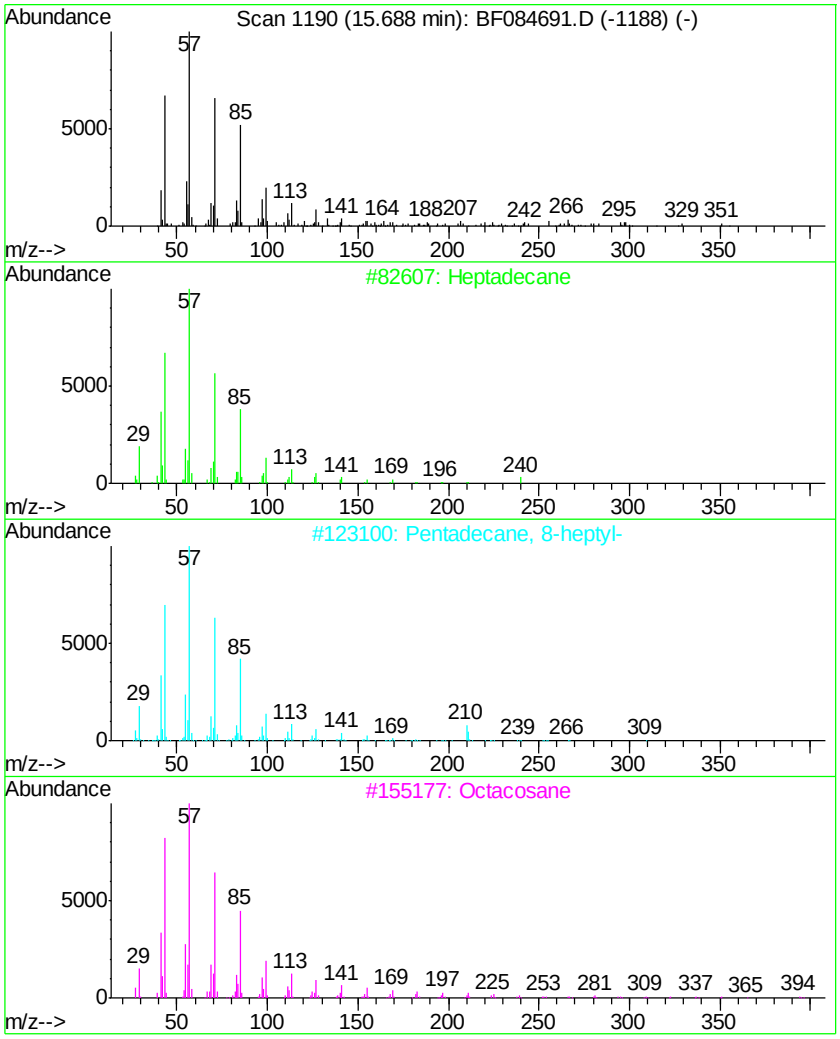
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

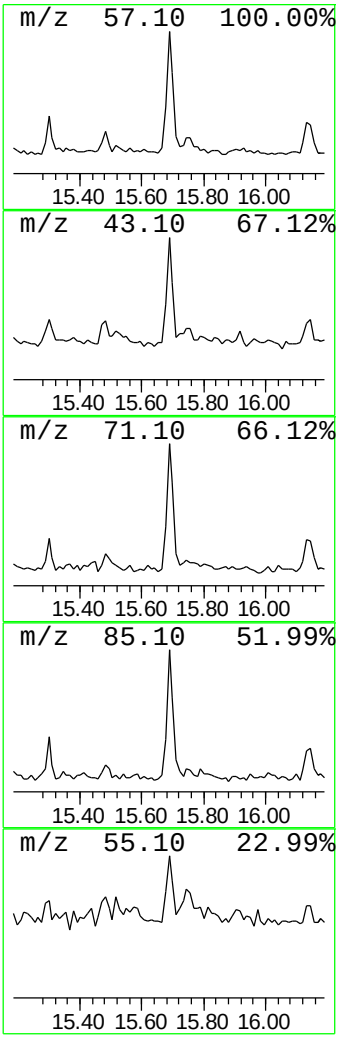
****

Peak Number 8 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.69	2.90 ng	162151	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	86
3	Octacosane	394	C28H58	000630-02-4	86
4	Pentacosane	352	C25H52	000629-99-2	86
5	Tetratriacontane	479	C34H70	014167-59-0	86





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Acq On : 30 Jan 2016 17:36
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Sample : H1261-09 5X
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SCARBOROUGH1516-00(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

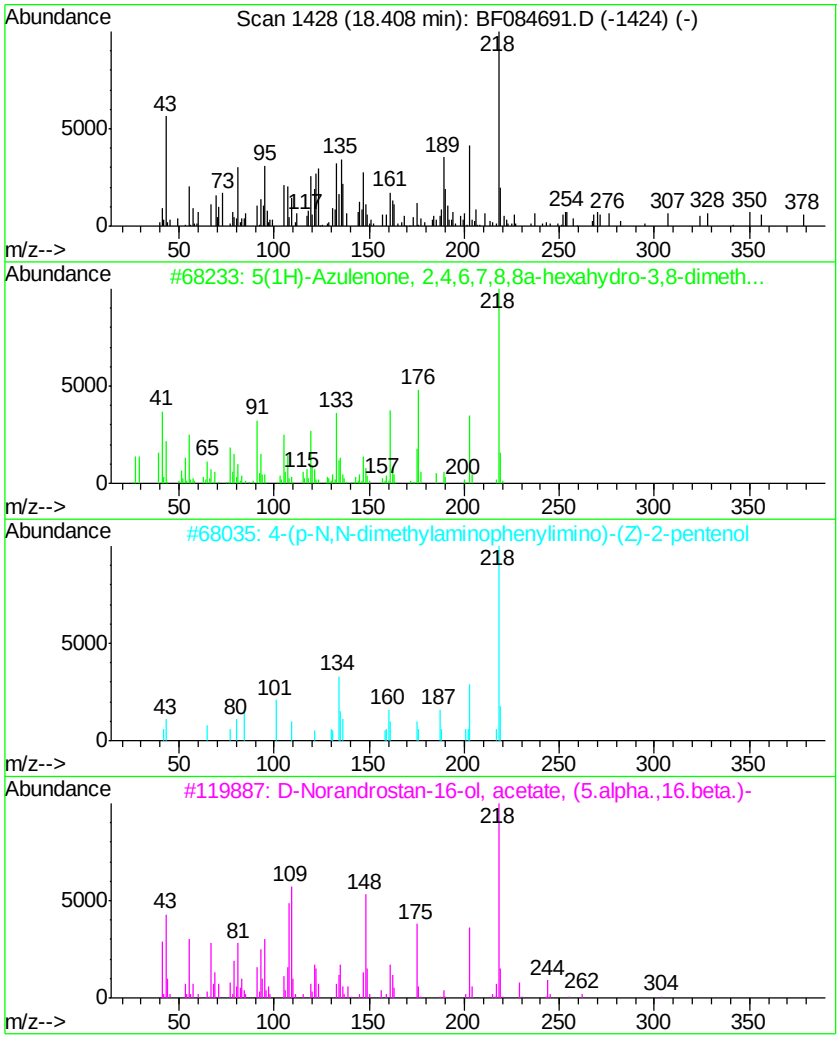
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

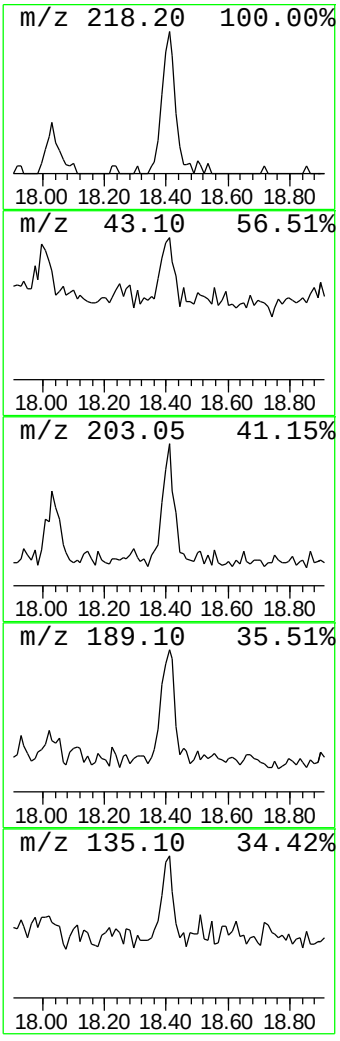
****

Peak Number 10 unknown18.41 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.41	3.44 ng	192906	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5(1H)-Azulenone, 2,4,6,7,8,8a-he...	218	C15H22O	006754-66-1	49
2	4-(p-N,N-dimethylaminophenylimin...	218	C13H18N2O	1000100-07-8	47
3	D-Norandrostan-16-ol, acetate, (...	304	C20H32O2	054411-62-0	47
4	D-Norandrostan-16-one, (5.alpha.)-	260	C18H28O	032319-06-5	47
5	D-Norandrostan-16-ol, (5.alpha.,...	262	C18H30O	035575-61-2	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF013016\
Data File : BF084691.D
Acq On : 30 Jan 2016 17:36
Operator : SJ/IZ
Sample : H1261-09 5X
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SCARBOROUGH1516-00(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one, 4...	4.18	2.1	ng	118087	1	6.73	1140240	20.0
2-Pentanone, 4-hy...	4.88	23.7	ng	1351710	1	6.73	1140240	20.0
unknown6.49	6.49	18.8	ng	1071460	1	6.73	1140240	20.0
1-Hexadecanethiol	13.73	2.1	ng	144142	5	13.87	1347730	20.0
unknown14.39	14.39	2.1	ng	142612	5	13.87	1347730	20.0
Heptadecane	15.69	2.9	ng	162151	6	15.27	1120050	20.0
unknown18.41	18.41	3.4	ng	192906	6	15.27	1120050	20.0