LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092225.D
Acq On : 12 Jan 2017 23:31
Operator : UM/SJ
Sample : I1030-19
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-0020

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-BF122116.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	4.721	245	248	264	rVB	910495	1358344	40.04%	4.114%
2	5.190	287	289	301	rBV	2834729	2975508	87.72%	9.013%
3	6.264	380	383	385	rBV	2417338	3392076	100.00%	10.274%
4	6.367	390	392	394	rBV	3620462	3338852	98.43%	10.113%
5	6.596	410	412	414	rBV	986466	1017245	29.99%	3.081%
6	6.744	423	425	428	rBV	2585078	2820567	83.15%	8.543%
7	7.167	459	462	464	rBV	2114926	2392435	70.53%	7.247%
8	7.876	522	524	527	rBV	1073995	1251438	36.89%	3.791%
9	8.962	616	619	621	rBV	3276184	3135953	92.45%	9.499%
10	9.362	652	654	656	rBV	308403	275694	8.13%	0.835%
11	9.579	671	673	675	rBV	42257	35012	1.03%	0.106%
12	9.625	675	677	680	rBV	1295335	1300666	38.34%	3.940%
13	10.082	713	717	718	rBV	62623	82035	2.42%	0.248%
14	10.299	733	736	737	rBV	25079	36907	1.09%	0.112%
15	10.413	744	746	749	rBV2	1728706	1939933	57.19%	5.876%
16	10.551	756	758	762	rBV	89353	112065	3.30%	0.339%
17	10.996	795	797	798	rBV	65357	62403	1.84%	0.189%
18	11.111	804	807	809	rBV	990758	1327760	39.14%	4.022%
19	11.659	852	855	859	rBV	111170	118763	3.50%	0.360%
20	12.528	929	931	934	rBV2	109384	117865	3.47%	0.357%
21	12.585	934	936	940	rBV2	40198	60436	1.78%	0.183%
22	12.688	943	945	948	rBV	2557059	2634204	77.66%	7.979%
23	12.939	963	967	969	rBV	54716	75045	2.21%	0.227%
24	13.236	990	993	994	rBV	49552	57091	1.68%	0.173%
25	13.282	994	997	1001	rVB2	32783	51453	1.52%	0.156%
26	13.602	1022	1025	1029	rBV	142542	224576	6.62%	0.680%
27	13.728	1034	1036	1039	rBV	840580	894832	26.38%	2.710%
28	13.922	1050	1053	1056	rBV	32252	37201	1.10%	0.113%
29	14.231	1077	1080	1086	rVB2	34466	68048	2.01%	0.206%
30	14.585	1108	1111	1113	rVB	68630	80466	2.37%	0.244%
31	14.642	1114	1116	1120	rBV	54149	55044	1.62%	0.167%
32	14.814	1128	1131	1132	rBV	68315	82132	2.42%	0.249%
33	14.848	1132	1134	1138	rVB3	24047	52470	1.55%	0.159%
34	15.088	1153	1155	1158	rBV	697432	855765	25.23%	2.592%

LSC Area Percent Report

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Operator : UM/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : COMP-0020

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-BF122116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.134	1158	1159	1162	rVB	34973	37267	1.10%	0.113%
36	15.500	1188	1191	1193	rBV	76929	110246	3.25%	0.334%
37	15.568	1193	1197	1199	rVV4	14328	39859	1.18%	0.121%
38	15.911	1225	1227	1234	rBV2	27130	48969	1.44%	0.148%
39	16.151	1246	1248	1252	rVB3	23269	47831	1.41%	0.145%
40	16.403	1268	1270	1272	rBV	24631	43015	1.27%	0.130%
41	16.551	1280	1283	1284	rBV2	31837	61944	1.83%	0.188%
42	16.585	1284	1286	1291	rVB	72182	136281	4.02%	0.413%
43	16.814	1303	1306	1312	rVB4	29371	72616	2.14%	0.220%
44	16.974	1318	1320	1326	rVB4	20027	47599	1.40%	0.144%
45	17.648	1376	1379	1385	rVB3	19584	48636	1.43%	0.147%

Sum of corrected areas: 33014547

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
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Misc :
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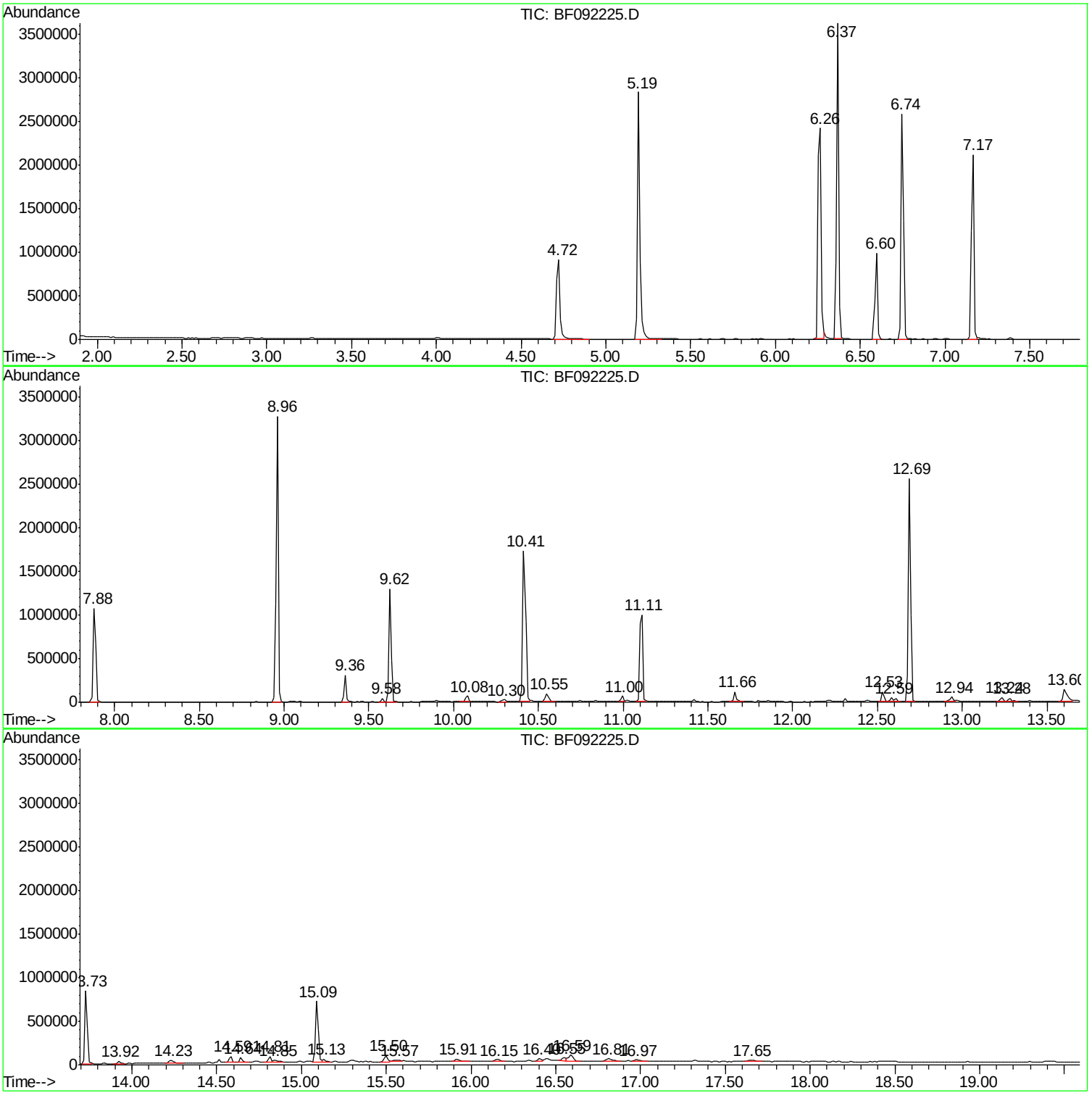
Instrument : BNA_F
ClientSampleId : COMP-0020

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092225.D
Acq On : 12 Jan 2017 23:31
Operator : UM/SJ
Sample : I1030-19
Misc :
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Instrument : BNA_F
ClientSampleId : COMP-0020

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

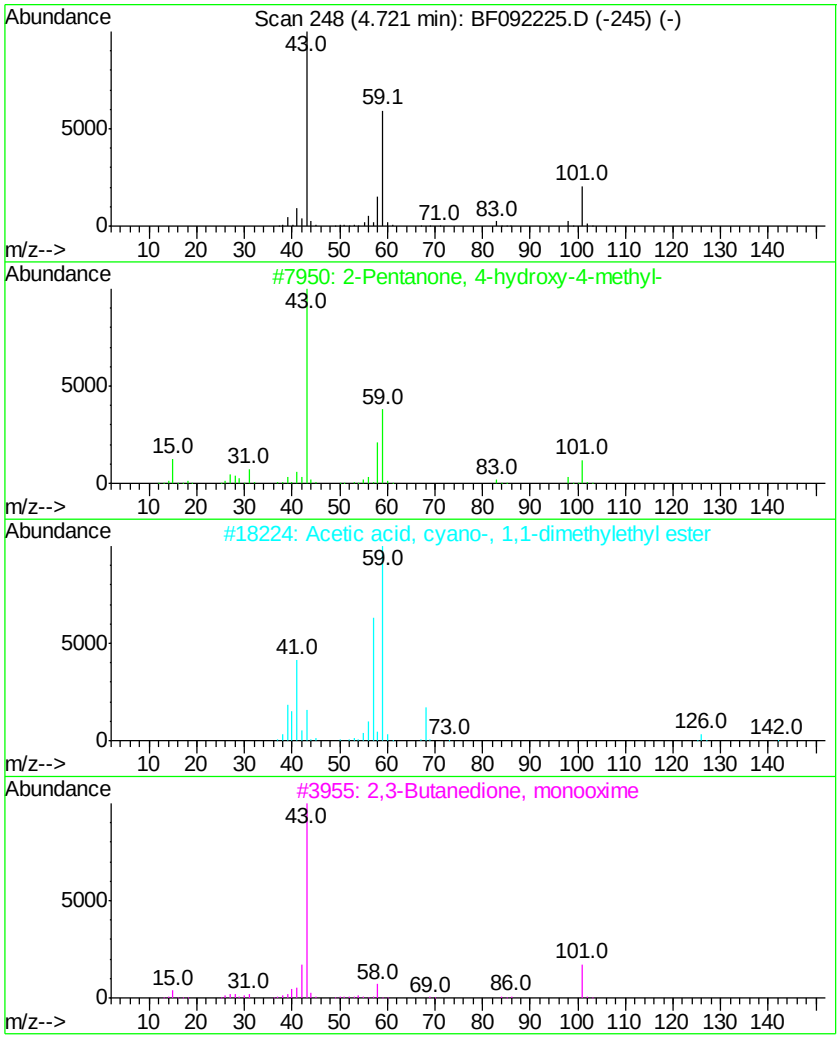
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

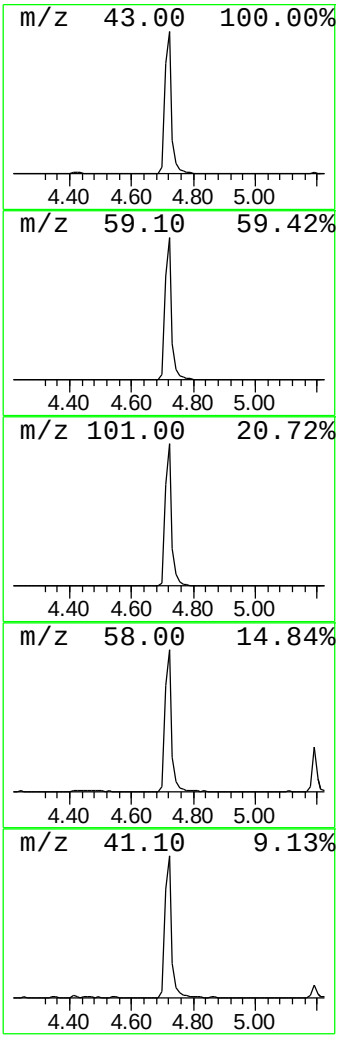
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.72	26.71 ng	1358340	1,4-Dichlorobenzene-d4	6.60

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	17
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9





Library Search Compound Report

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Data File : BF092225.D
Acq On : 12 Jan 2017 23:31
Operator : UM/SJ
Sample : I1030-19
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-0020

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

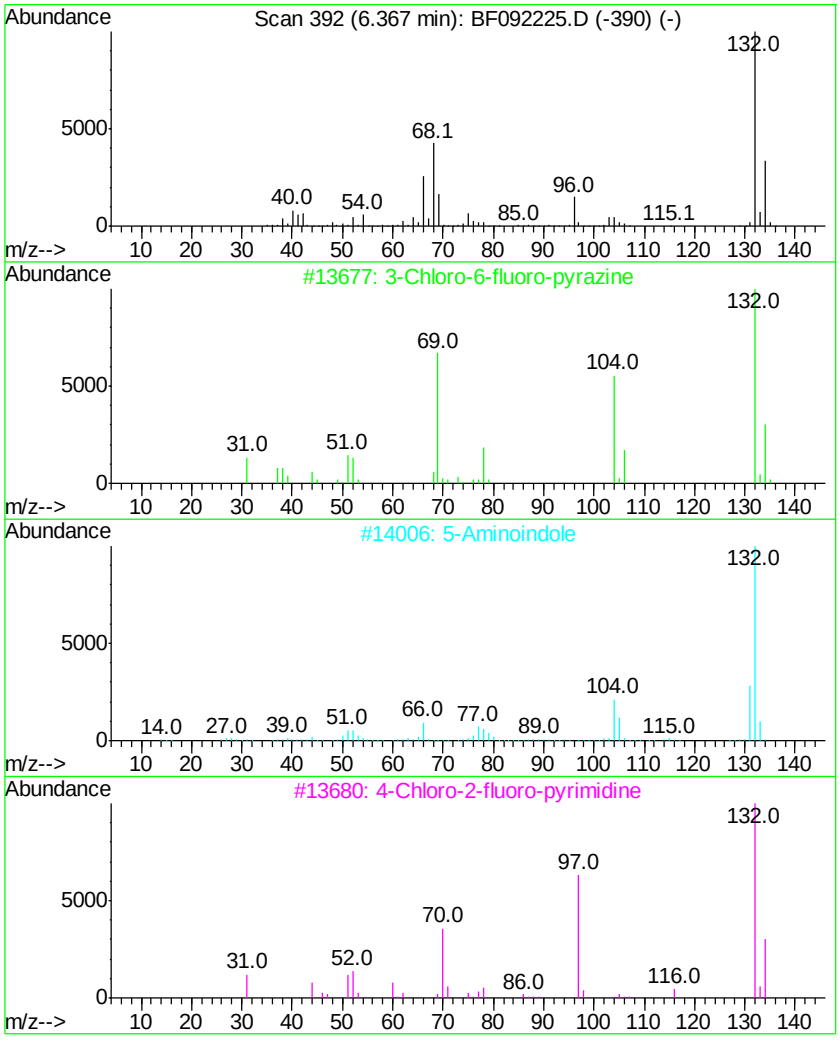
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

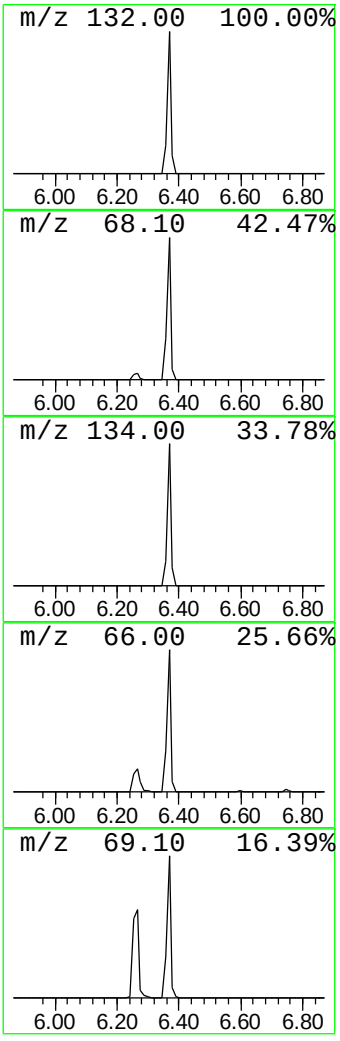
****

Peak Number 2 unknown6.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.37	65.65 ng	3338850	1,4-Dichlorobenzene-d4	6.60

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	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Sample : I1030-19
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Instrument : BNA_F
ClientSampleId : COMP-0020

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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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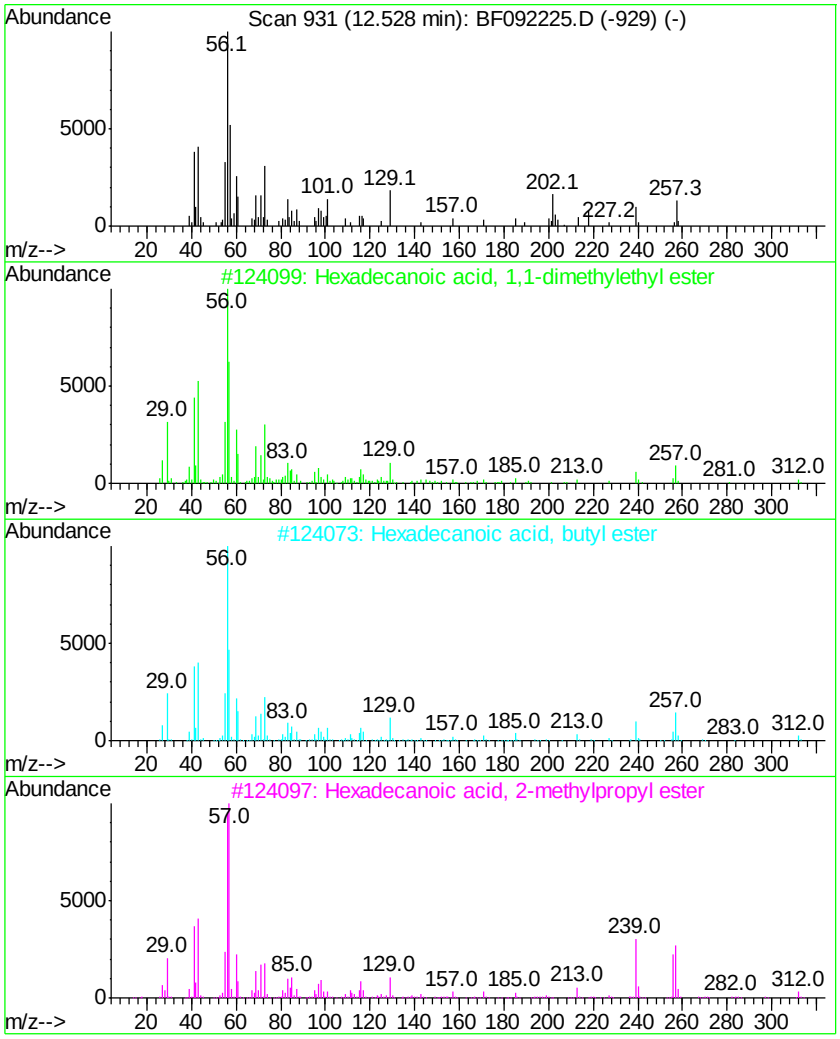
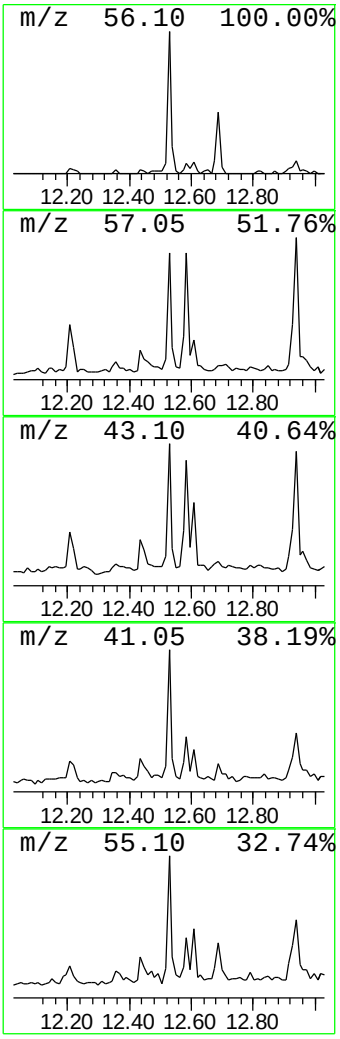
Peak Number 4 Hexadecanoic acid, 1,1-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.53	2.63 ng	117865	Chrysene-d12	13.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	90
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	83
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	42
4	1-Hexene, 4-methyl-	98	C7H14	003769-23-1	27
5	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092225.D
Acq On : 12 Jan 2017 23:31
Operator : UM/SJ
Sample : I1030-19
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-0020

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

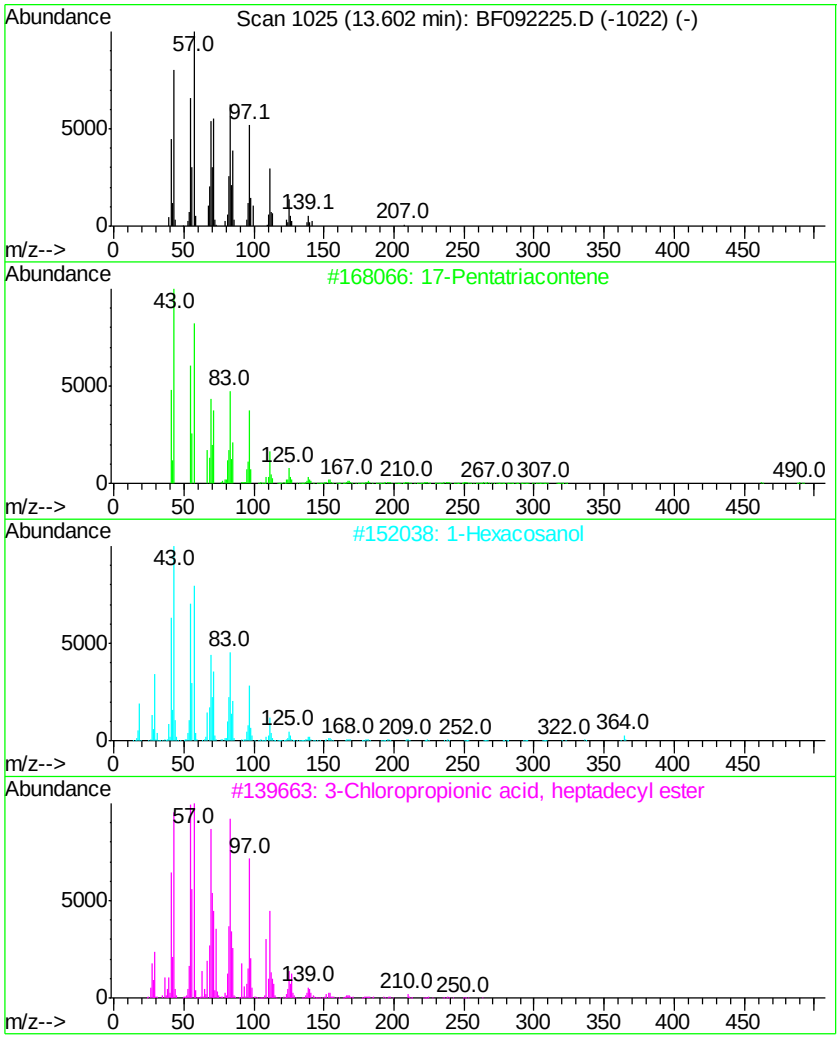
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

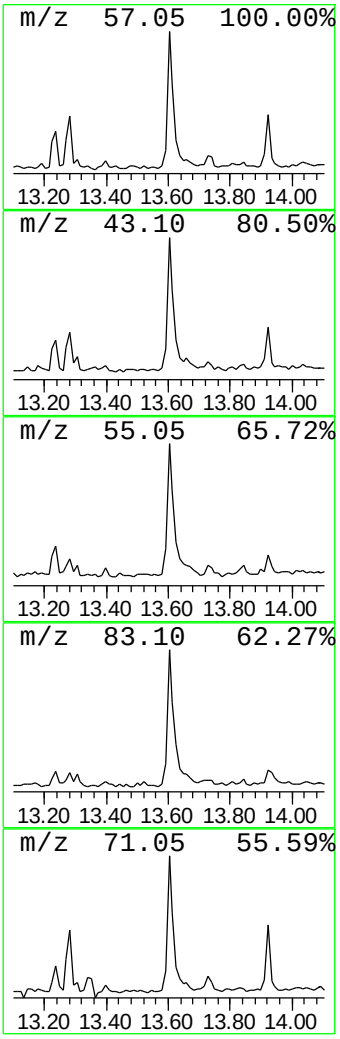
****

Peak Number 5 17-Pentatriacontene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.60	5.02 ng	224576	Chrysene-d12	13.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	90
2	1-Hexacosanol	382	C26H54O	000506-52-5	86
3	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	76
4	2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	72
5	1-Nonadecene	266	C19H38	018435-45-5	68





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Operator : UM/SJ
Sample : I1030-19
Misc :
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Instrument : BNA_F
ClientSampleId : COMP-0020

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

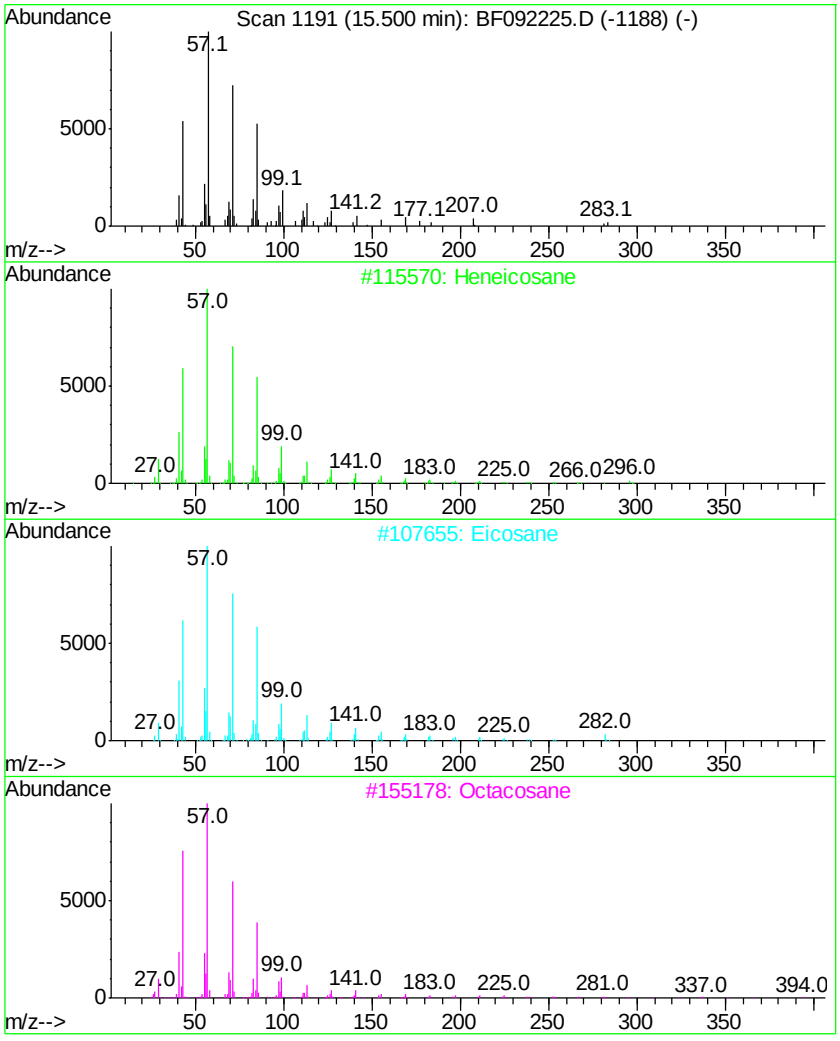
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

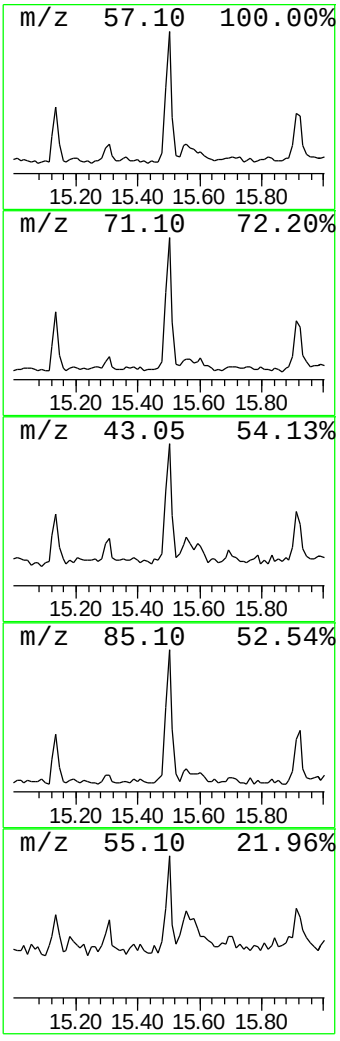
****

Peak Number 6 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.50	2.58 ng	110246	Perylene-d12	15.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Eicosane	282	C20H42	000112-95-8	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Nonacosane	408	C29H60	000630-03-5	90
5	Heptadecane	240	C17H36	000629-78-7	87





Library Search Compound Report

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Sample : I1030-19
Misc :
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Instrument : BNA_F
ClientSampleId : COMP-0020

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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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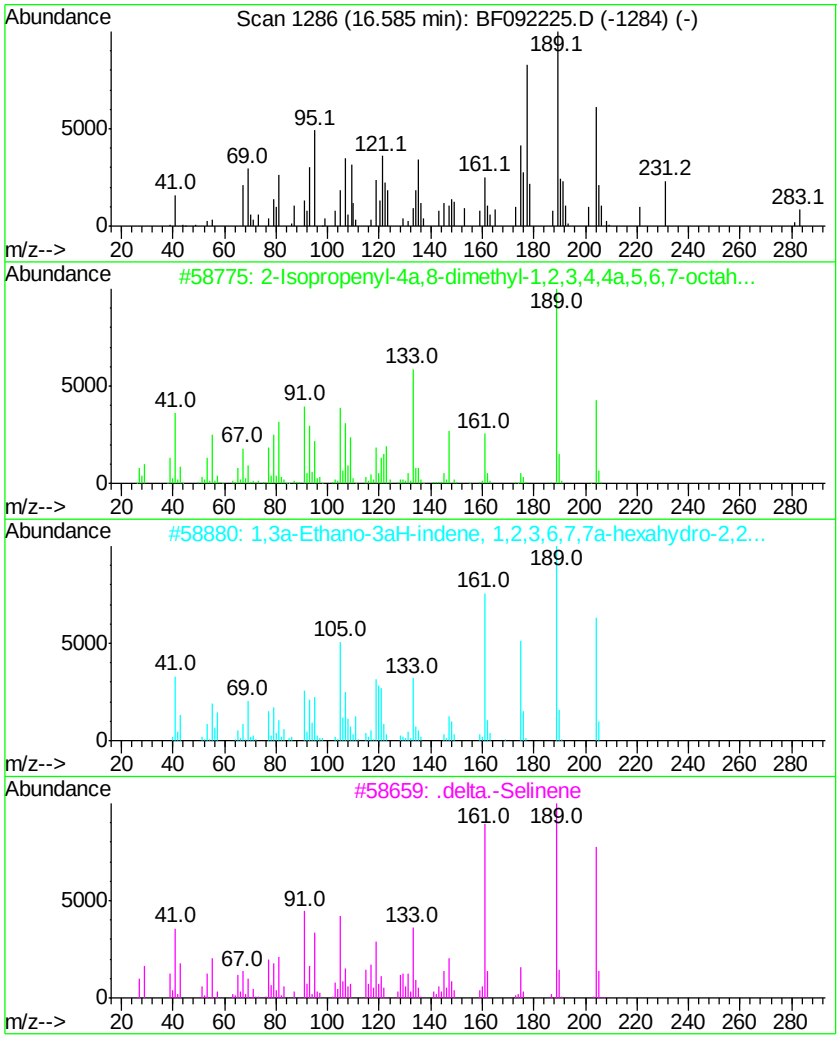
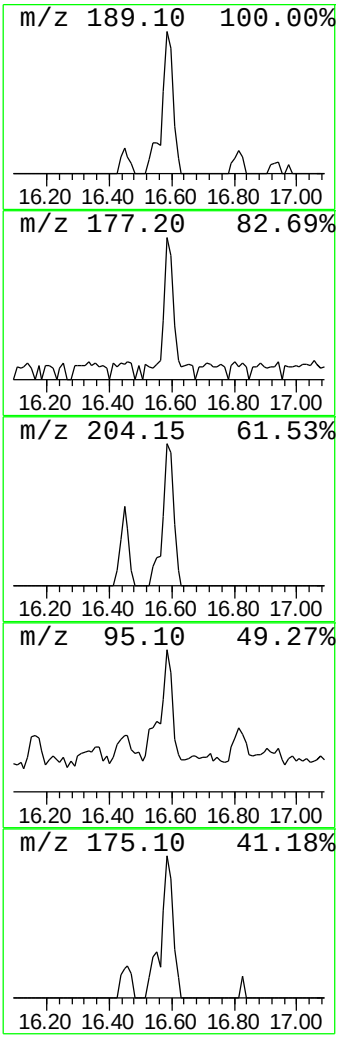
Peak Number 7 unknown16.59 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.59	3.19 ng	136281	Perylene-d12	15.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	1000192-43-5	42
2	1,3a-Ethano-3aH-indene, 1,2,3,6,...	204	C15H24	004545-68-0	38
3	.delta.-Selinene	204	C15H24	028624-23-9	35
4	1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	000489-29-2	30
5	Spiro[5.5]undec-2-ene, 3,7,7-tri...	204	C15H24	018431-82-8	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011217\
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ClientSampleId : COMP-0020

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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...	4.72	26.7	ng	1358340	1	6.60	1017250	20.0
unknown6.37	6.37	65.7	ng	3338850	1	6.60	1017250	20.0
Hexadecanoic acid...	12.53	2.6	ng	117865	5	13.73	894832	20.0
17-Pentatriacontene	13.60	5.0	ng	224576	5	13.73	894832	20.0
Heneicosane	15.50	2.6	ng	110246	6	15.09	855765	20.0
unknown16.59	16.59	3.2	ng	136281	6	15.09	855765	20.0