LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100217\
Data File : BF099022.D
Acq On : 3 Oct 2017 1:38
Operator : SJ/JU
Sample : I5531-09 5X
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-62A-0-2.5

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-BF092317.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	2.175	12	15	23	rVB2	42171	70848	8.98%	0.811%
2	4.504	408	411	420	rBV	130714	150988	19.15%	1.729%
3	5.122	512	516	533	rBV	735082	788630	100.00%	9.030%
4	5.516	581	583	590	rVB	19508	17684	2.24%	0.202%
5	6.522	750	754	762	rBV	293489	258557	32.79%	2.961%
6	6.669	776	779	784	rVB	78873	59360	7.53%	0.680%
7	6.904	815	819	823	rBV	804346	632584	80.21%	7.244%
8	6.957	825	828	832	rVB	27457	21944	2.78%	0.251%
9	7.057	841	845	849	rBV	503754	418439	53.06%	4.791%
10	7.463	910	914	917	rBV	304884	263500	33.41%	3.017%
11	8.157	1029	1032	1033	rBV	11668	10230	1.30%	0.117%
12	8.186	1033	1037	1040	rVV	905251	737711	93.54%	8.447%
13	8.239	1042	1046	1048	rVB2	27877	28583	3.62%	0.327%
14	8.469	1076	1085	1090	rBV7	16210	26860	3.41%	0.308%
15	8.598	1104	1107	1109	rBV	34487	25624	3.25%	0.293%
16	8.686	1120	1122	1125	rBV4	12931	11986	1.52%	0.137%
17	8.727	1125	1129	1131	rVV5	8448	10524	1.33%	0.121%
18	8.769	1133	1136	1140	rVV2	22076	20686	2.62%	0.237%
19	8.863	1150	1152	1156	rVB3	11618	14480	1.84%	0.166%
20	8.898	1156	1158	1162	rVB	22626	18048	2.29%	0.207%
21	8.957	1166	1168	1171	rBV4	8299	10429	1.32%	0.119%
22	8.998	1171	1175	1178	rVV2	25411	26433	3.35%	0.303%
23	9.086	1188	1190	1194	rVB2	15268	15893	2.02%	0.182%
24	9.127	1194	1197	1199	rBV2	11129	12866	1.63%	0.147%
25	9.198	1207	1209	1215	rVB	45038	35480	4.50%	0.406%
26	9.257	1215	1219	1224	rBV	604469	482649	61.20%	5.527%
27	9.333	1229	1232	1236	rBV3	26085	31273	3.97%	0.358%
28	9.410	1243	1245	1247	rVB2	12815	11014	1.40%	0.126%
29	9.457	1250	1253	1257	rBV	11417	13291	1.69%	0.152%
30	9.527	1261	1265	1269	rBV	37598	51711	6.56%	0.592%
31	9.598	1274	1277	1280	rBV	43619	48479	6.15%	0.555%
32	9.651	1283	1286	1289	rVB	120805	105288	13.35%	1.206%
33	9.716	1294	1297	1299	rBV	22667	20143	2.55%	0.231%
34	9.804	1309	1312	1315	rVB2	23611	21929	2.78%	0.251%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100217\
Data File : BF099022.D
Acq On : 3 Oct 2017 1:38
Operator : SJ/JU
Sample : I5531-09 5X
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-62A-0-2.5

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-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.857	1317	1321	1326	rVB3	17658	27385	3.47%	0.314%
36	9.945	1330	1336	1339	rVV	766728	668276	84.74%	7.652%
37	9.974	1339	1341	1345	rVV3	19636	25114	3.18%	0.288%
38	10.045	1349	1353	1357	rBV2	21401	30067	3.81%	0.344%
39	10.086	1357	1360	1364	rBV5	10163	13313	1.69%	0.152%
40	10.139	1364	1369	1373	rVB3	30078	39672	5.03%	0.454%
41	10.186	1373	1377	1381	rBV2	33180	37341	4.73%	0.428%
42	10.257	1386	1389	1391	rBV	26379	24583	3.12%	0.281%
43	10.286	1391	1394	1396	rBV	19409	14338	1.82%	0.164%
44	10.351	1400	1405	1406	rBV3	25465	33236	4.21%	0.381%
45	10.363	1406	1407	1410	rVB2	31159	17729	2.25%	0.203%
46	10.439	1414	1420	1422	rVB7	8536	12742	1.62%	0.146%
47	10.492	1422	1429	1431	rBV3	15385	28055	3.56%	0.321%
48	10.580	1441	1444	1450	rVB2	52581	60457	7.67%	0.692%
49	10.633	1450	1453	1459	rVB6	10251	14115	1.79%	0.162%
50	10.851	1484	1490	1493	rBV2	93414	107052	13.57%	1.226%
51	11.027	1516	1520	1523	rBV4	12764	18202	2.31%	0.208%
52	11.063	1523	1526	1530	rVV5	15436	19496	2.47%	0.223%
53	11.180	1540	1546	1552	rBV10	10570	25887	3.28%	0.296%
54	11.286	1560	1564	1566	rBV2	21234	21585	2.74%	0.247%
55	11.315	1566	1569	1575	rVB2	47977	56343	7.14%	0.645%
56	11.380	1575	1580	1585	rVB5	7699	13884	1.76%	0.159%
57	11.433	1585	1589	1591	rBV	740168	639377	81.07%	7.321%
58	11.457	1591	1593	1595	rVB	45384	35610	4.52%	0.408%
59	11.662	1625	1628	1631	rBV3	16741	15344	1.95%	0.176%
60	11.710	1634	1636	1639	rVV2	15273	11880	1.51%	0.136%
61	11.762	1643	1645	1650	rVB3	14322	16064	2.04%	0.184%
62	11.839	1655	1658	1662	rBV5	7961	13892	1.76%	0.159%
63	11.933	1671	1674	1676	rBV	17380	17937	2.27%	0.205%
64	11.962	1677	1679	1684	rVB2	21380	17878	2.27%	0.205%
65	12.039	1690	1692	1695	rBV2	14031	13953	1.77%	0.160%
66	12.115	1703	1705	1709	rBV2	14707	15952	2.02%	0.183%
67	12.227	1722	1724	1726	rBV2	12829	11080	1.40%	0.127%
68	12.251	1726	1728	1732	rVV4	9245	10430	1.32%	0.119%
69	12.357	1743	1746	1751	rBV6	11078	18501	2.35%	0.212%
70	12.404	1751	1754	1756	rBV3	12430	14331	1.82%	0.164%
71	12.480	1764	1767	1769	rBV3	21588	20876	2.65%	0.239%

LSC Area Percent Report

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Data File : BF099022.D
Acq On : 3 Oct 2017 1:38
Operator : SJ/JU
Sample : I5531-09 5X
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-62A-0-2.5

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-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	12.509	1769	1772	1775	rVB3	18744	19716	2.50%	0.226%
73	12.645	1792	1795	1798	rBV	66516	56760	7.20%	0.650%
74	12.821	1823	1825	1828	rVB3	13948	10463	1.33%	0.120%
75	12.874	1831	1834	1836	rBV	81975	91881	11.65%	1.052%
76	13.009	1854	1857	1861	rBV	536121	445772	56.52%	5.104%
77	13.233	1892	1895	1897	rBV2	19733	20766	2.63%	0.238%
78	13.486	1935	1938	1943	rBV	68863	56938	7.22%	0.652%
79	14.074	2034	2038	2041	rBV	834315	738650	93.66%	8.458%
80	15.568	2288	2292	2300	rVB	488197	635926	80.64%	7.282%

Sum of corrected areas: 8732993

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Data File : BF099022.D
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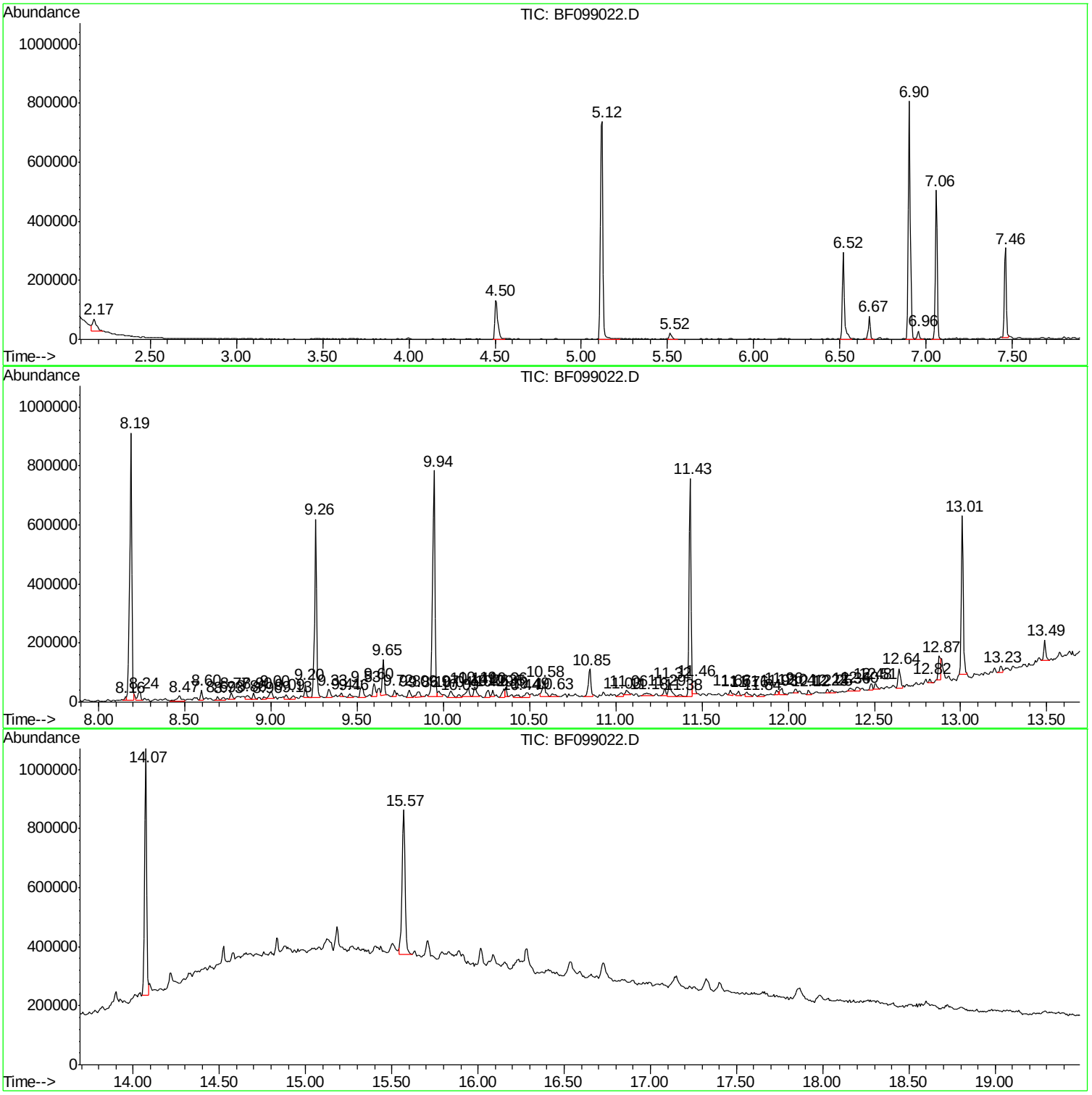
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G-62A-0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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\BF100217\
Data File : BF099022.D
Acq On : 3 Oct 2017 1:38
Operator : SJ/JU
Sample : I5531-09 5X
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-62A-0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

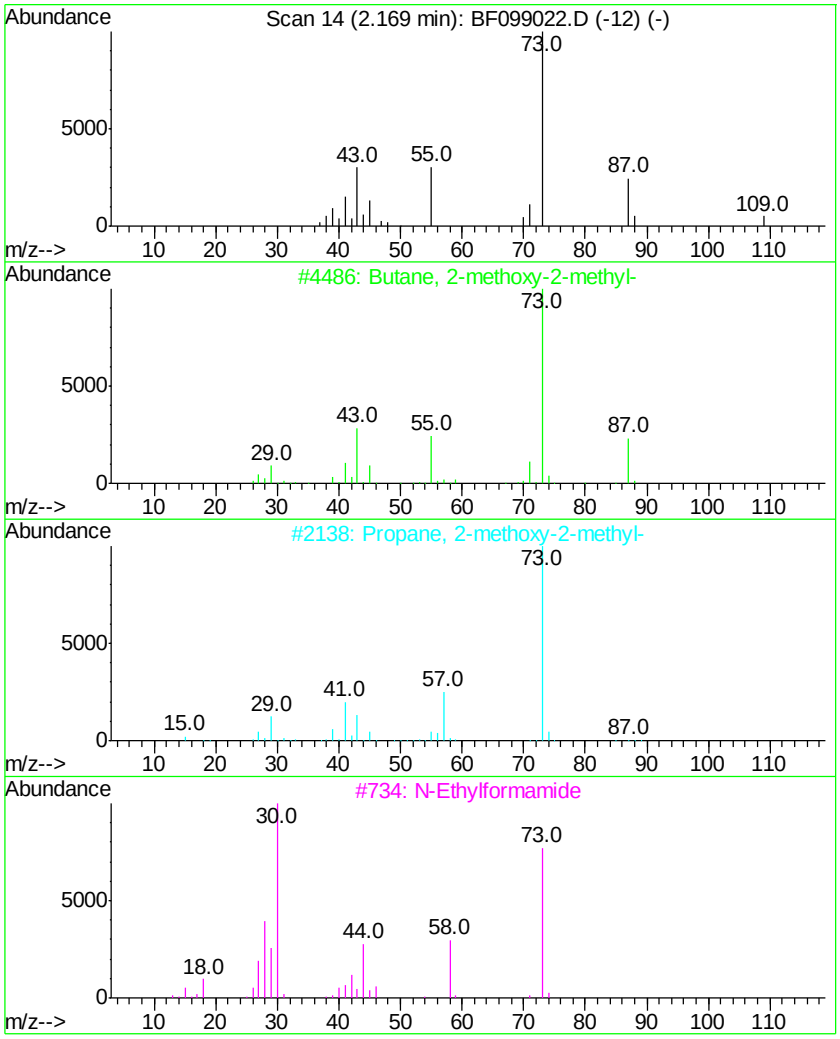
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

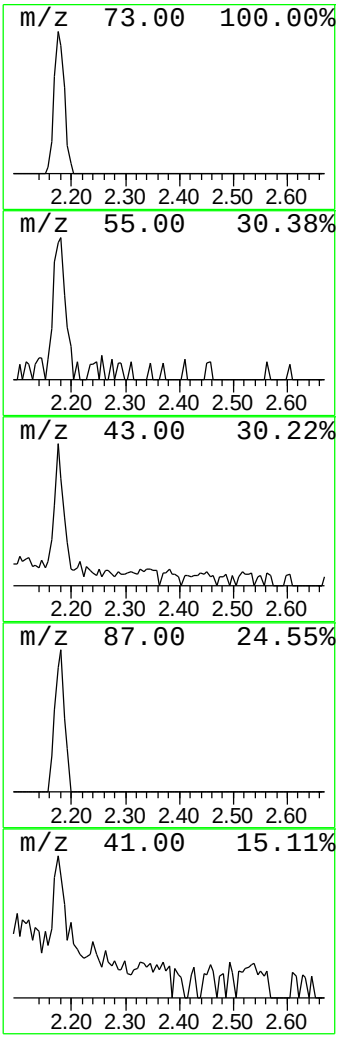
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	2.24 ng	70848	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
3	N-Ethylformamide	73	C3H7NO	000627-45-2	5
4	Formamide, N,N-dimethyl-	73	C3H7NO	000068-12-2	5
5	1,3-Dioxolane	74	C3H6O2	000646-06-0	4





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100217\
Data File : BF099022.D
Acq On : 3 Oct 2017 1:38
Operator : SJ/JU
Sample : I5531-09 5X
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-62A-0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

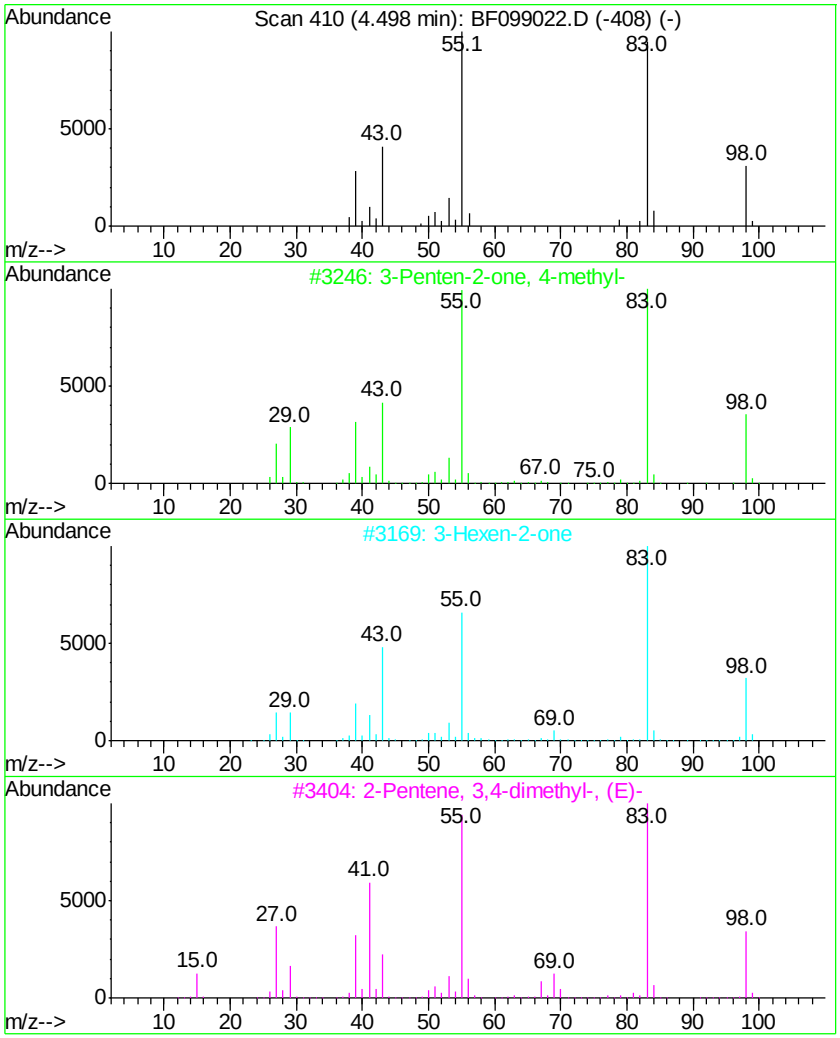
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

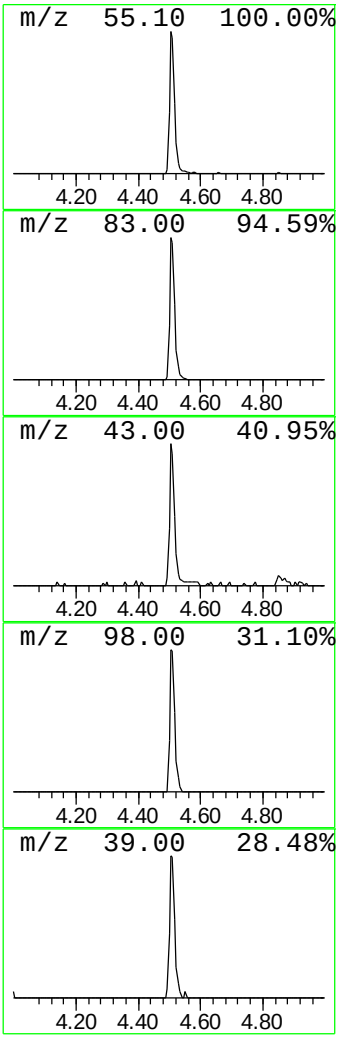
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.50	4.77 ng	150988	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	90
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





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Operator : SJ/JU
Sample : I5531-09 5X
Misc :
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Instrument : BNA_F
ClientSampleId : G-62A-0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

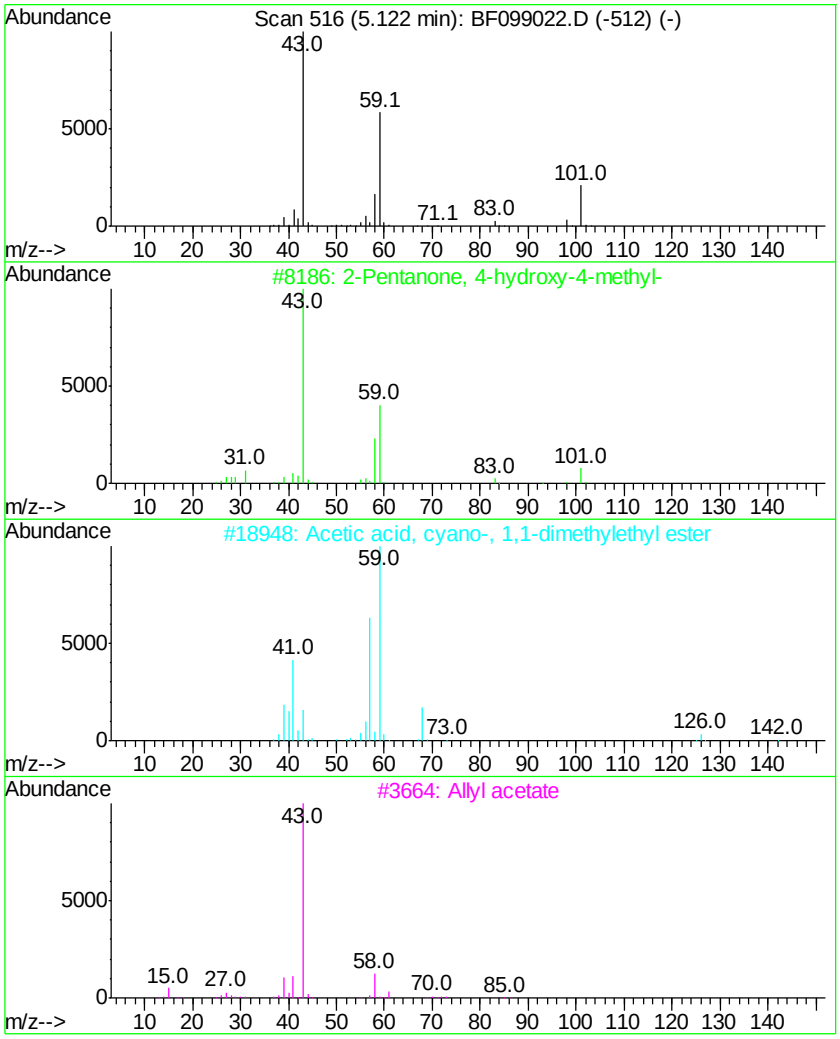
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

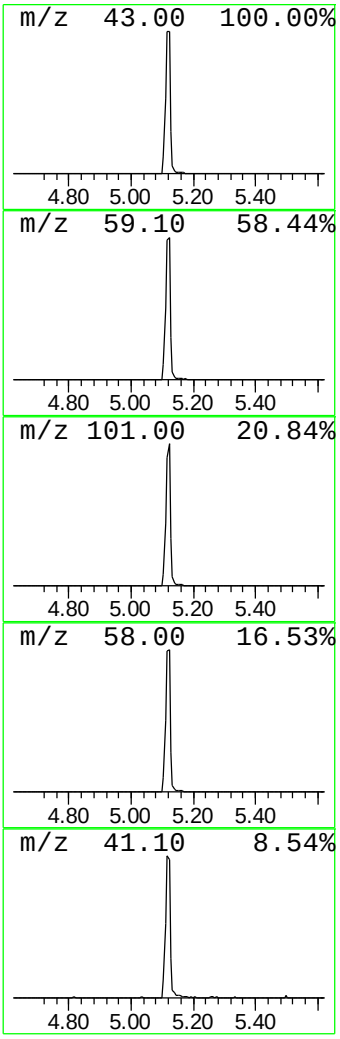
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	24.93 ng	788630	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	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Allyl acetate	100	C5H8O2	000591-87-7	9
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

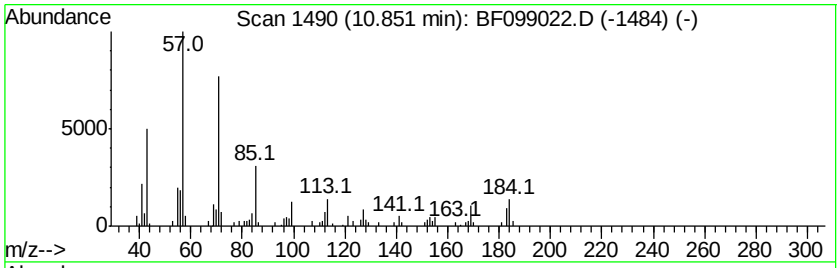
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

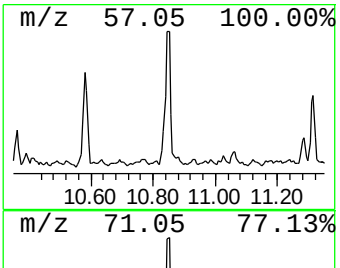
****

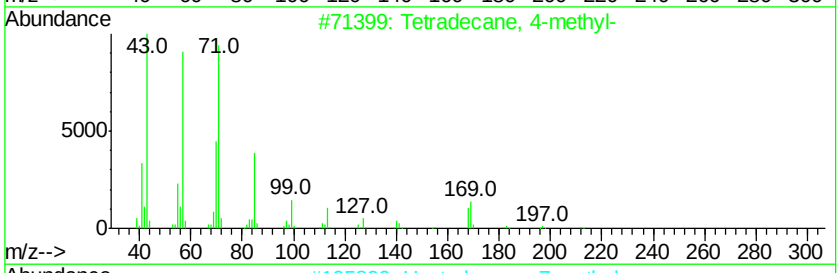
Peak Number 5 Tetradecane, 4-methyl- Concentration Rank 4

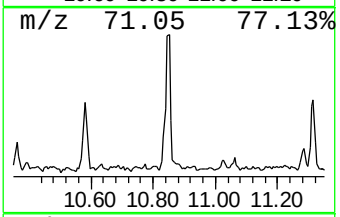
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.85	3.35 ng	107052	Phenanthrene-d10	11.43

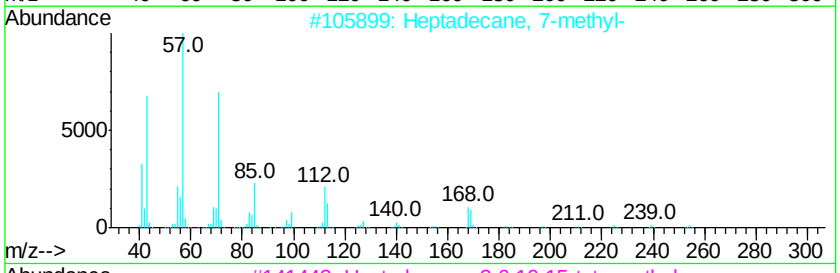
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane, 4-methyl-	212	C15H32	025117-24-2	80
2	Heptadecane, 7-methyl-	254	C18H38	020959-33-5	80
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	72
4	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	64
5	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	64

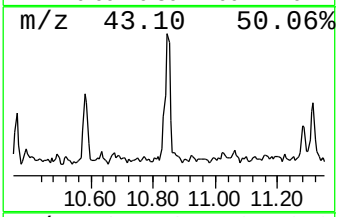


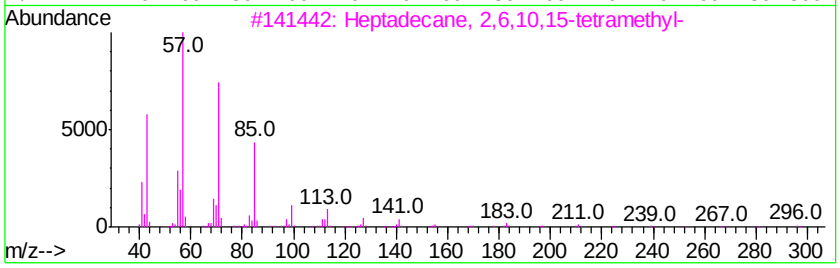


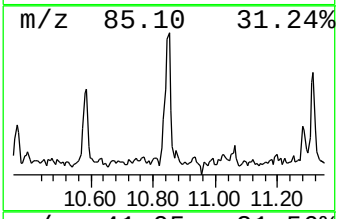


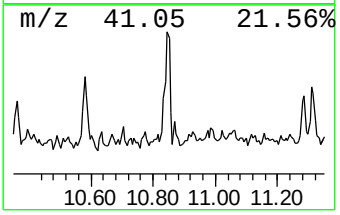












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100217\
Data File : BF099022.D
Acq On : 3 Oct 2017 1:38
Operator : SJ/JU
Sample : I5531-09 5X
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-62A-0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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
Butane, 2-methoxy...	2.17	2.2	ng	70848	1	6.90	632584	20.0
3-Penten-2-one, 4...	4.50	4.8	ng	150988	1	6.90	632584	20.0
2-Pentanone, 4-hy...	5.12	24.9	ng	788630	1	6.90	632584	20.0
Tetradecane, 4-me...	10.85	3.4	ng	107052	4	11.43	639377	20.0