LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100617\
Data File : BF099177.D
Acq On : 7 Oct 2017 5:39
Operator : SJ/JU
Sample : I5542-07
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OWL-C8-GW

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	2.169	9	14	22	rVB	620514	793939	20.61%	2.904%
2	5.093	507	511	527	rVB	221015	274954	7.14%	1.006%
3	5.487	574	578	581	rBV	2055199	1858593	48.25%	6.799%
4	6.492	744	749	759	rBV	1301287	1228921	31.90%	4.496%
5	6.634	768	773	776	rBV	3047423	2958118	76.80%	10.821%
6	6.863	808	812	815	rBV	961162	761477	19.77%	2.786%
7	7.022	834	839	842	rBV	2867981	2659544	69.04%	9.729%
8	7.428	903	908	911	rVB	2050291	2186142	56.75%	7.997%
9	7.875	981	984	988	rBV	42811	40749	1.06%	0.149%
10	8.145	1025	1030	1033	rBV	1172780	1064468	27.63%	3.894%
11	8.339	1058	1063	1066	rBV	72046	65386	1.70%	0.239%
12	8.863	1146	1152	1159	rBV6	33368	55933	1.45%	0.205%
13	9.063	1178	1186	1188	rBV4	26431	52802	1.37%	0.193%
14	9.222	1207	1213	1216	rBV	3836483	3851930	100.00%	14.091%
15	9.563	1266	1271	1275	rBV5	22600	43707	1.13%	0.160%
16	9.610	1275	1279	1282	rBV	228486	182733	4.74%	0.668%
17	9.816	1310	1314	1317	rVB4	35234	49768	1.29%	0.182%
18	9.898	1317	1328	1332	rBV	1347608	1218923	31.64%	4.459%
19	10.310	1395	1398	1403	rVB2	175376	182521	4.74%	0.668%
20	10.627	1448	1452	1456	rBV	177067	207251	5.38%	0.758%
21	10.692	1458	1463	1466	rBV	2005750	2000489	51.93%	7.318%
22	10.792	1477	1480	1489	rVB3	67593	92894	2.41%	0.340%
23	11.386	1577	1581	1584	rBV	1237277	1052860	27.33%	3.851%
24	11.904	1666	1669	1673	rBV	68205	63721	1.65%	0.233%
25	11.998	1682	1685	1690	rVB2	31531	39618	1.03%	0.145%
26	12.598	1784	1787	1791	rBV	49073	46833	1.22%	0.171%
27	12.968	1845	1850	1853	rBV	2805279	2819325	73.19%	10.313%
28	13.851	1997	2000	2004	rBV	71741	73603	1.91%	0.269%
29	14.021	2025	2029	2037	rVB	729418	644476	16.73%	2.358%
30	15.492	2274	2279	2289	rVB2	499789	637743	16.56%	2.333%
31	17.121	2551	2556	2564	rVV7	36184	75109	1.95%	0.275%
32	17.721	2651	2658	2667	rVB7	20169	52086	1.35%	0.191%

LSC Area Percent Report

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Data File : BF099177.D
Acq On : 7 Oct 2017 5:39
Operator : SJ/JU
Sample : I5542-07
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OWL-C8-GW

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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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

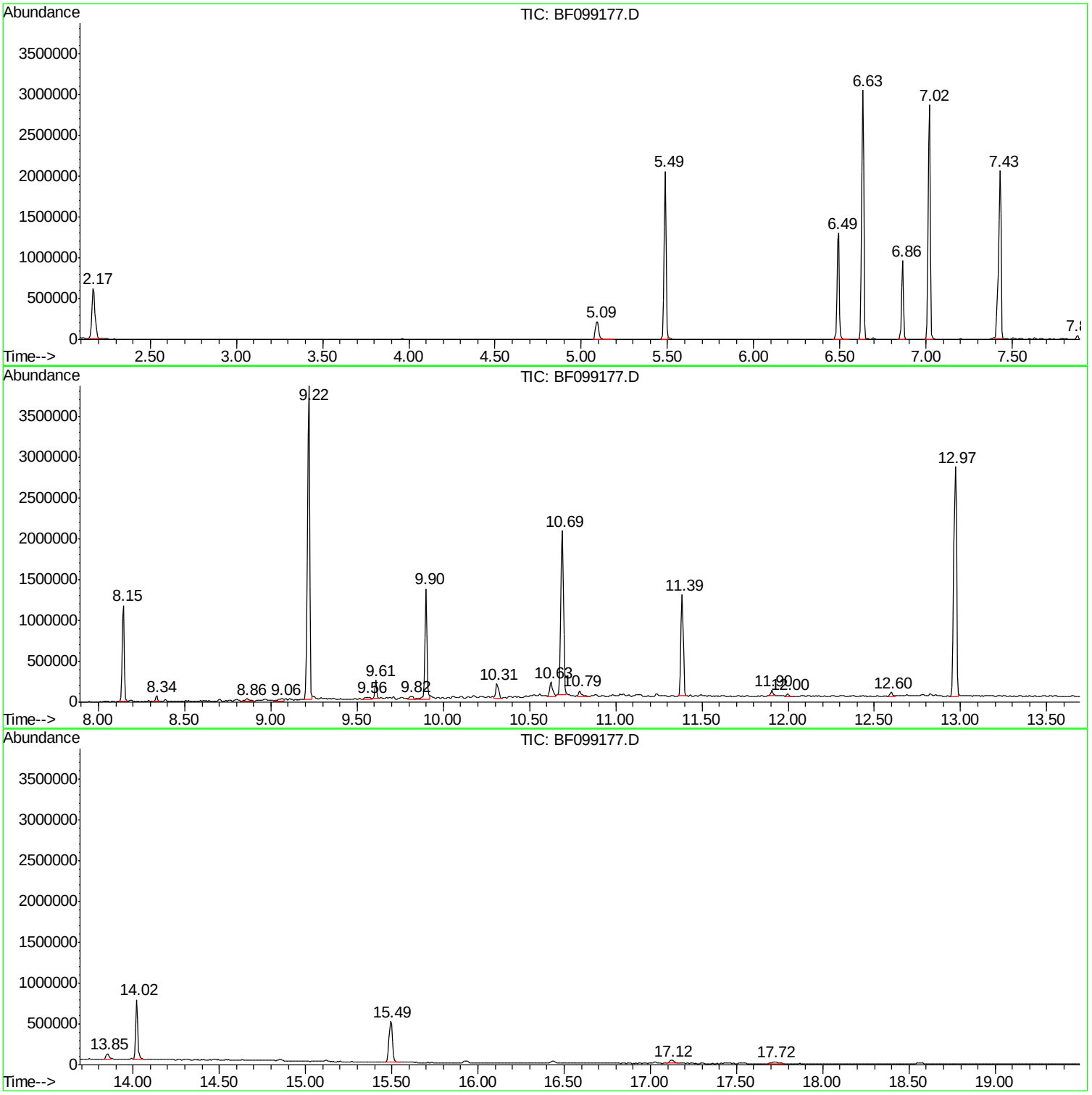
Sum of corrected areas: 27336616

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100617\
Data File : BF099177.D
Acq On : 7 Oct 2017 5:39
Operator : SJ/JU
Sample : I5542-07
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OWL-C8-GW

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



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Sample : I5542-07
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ClientSampleId : OWL-C8-GW

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

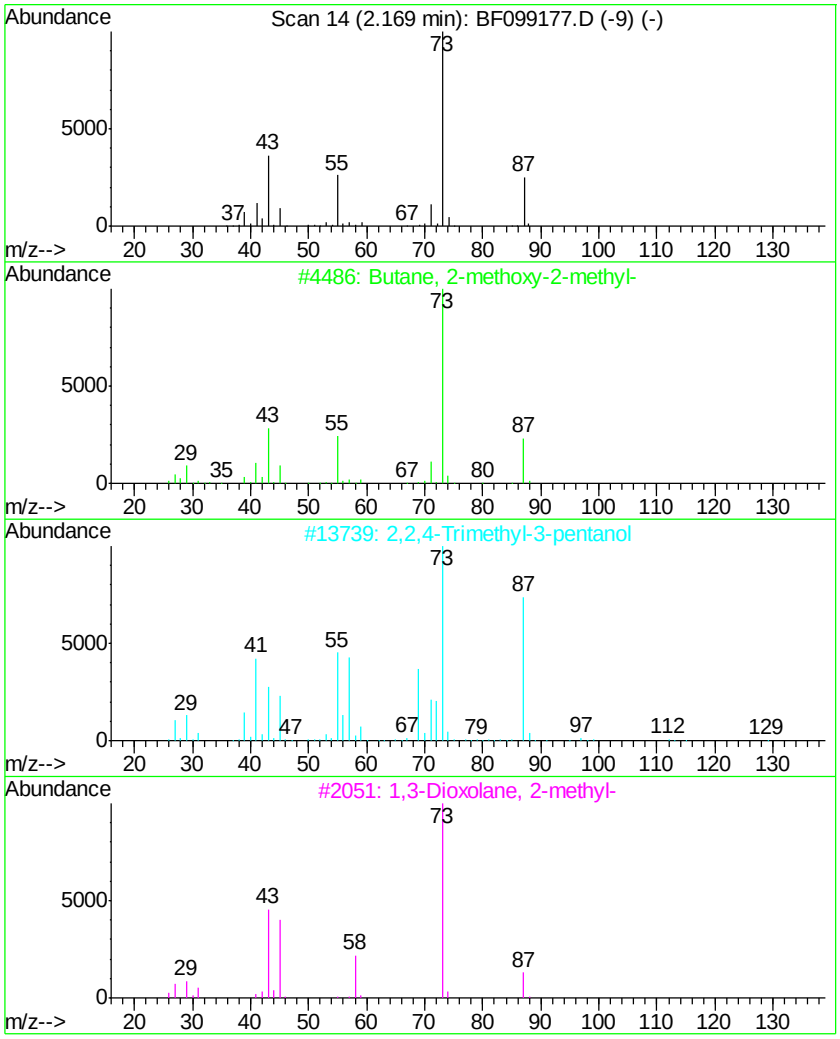
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

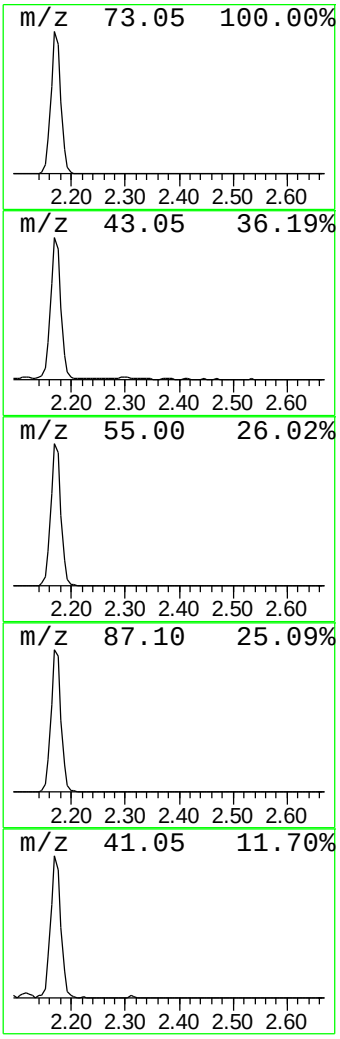
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	20.85 ng	793939	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12





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Operator : SJ/JU
Sample : I5542-07
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Instrument : BNA_F
ClientSampleId : OWL-C8-GW

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

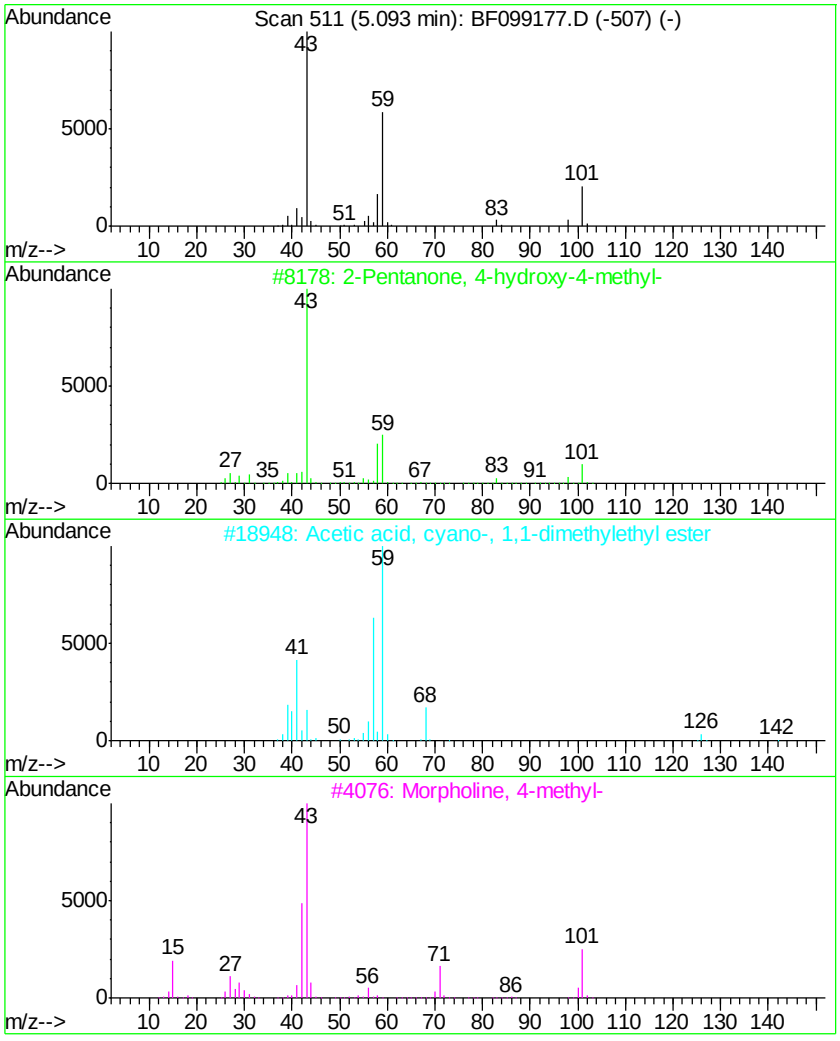
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

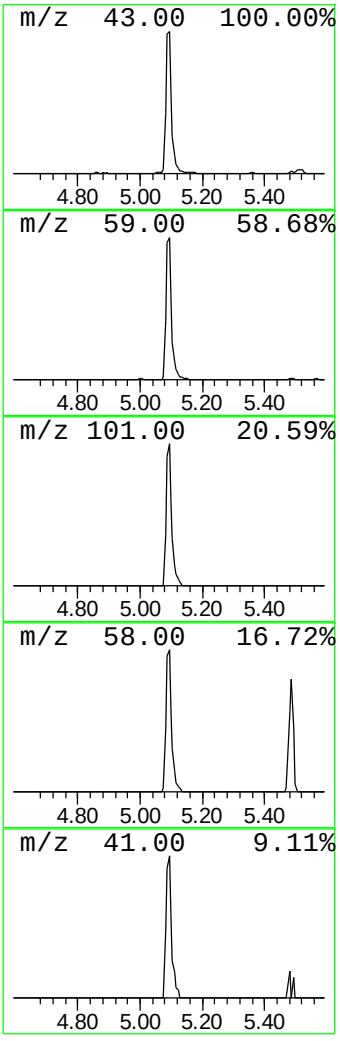
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	7.22 ng	274954	1,4-Dichlorobenzene-d4	6.86

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100617\
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Operator : SJ/JU
Sample : I5542-07
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OWL-C8-GW

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

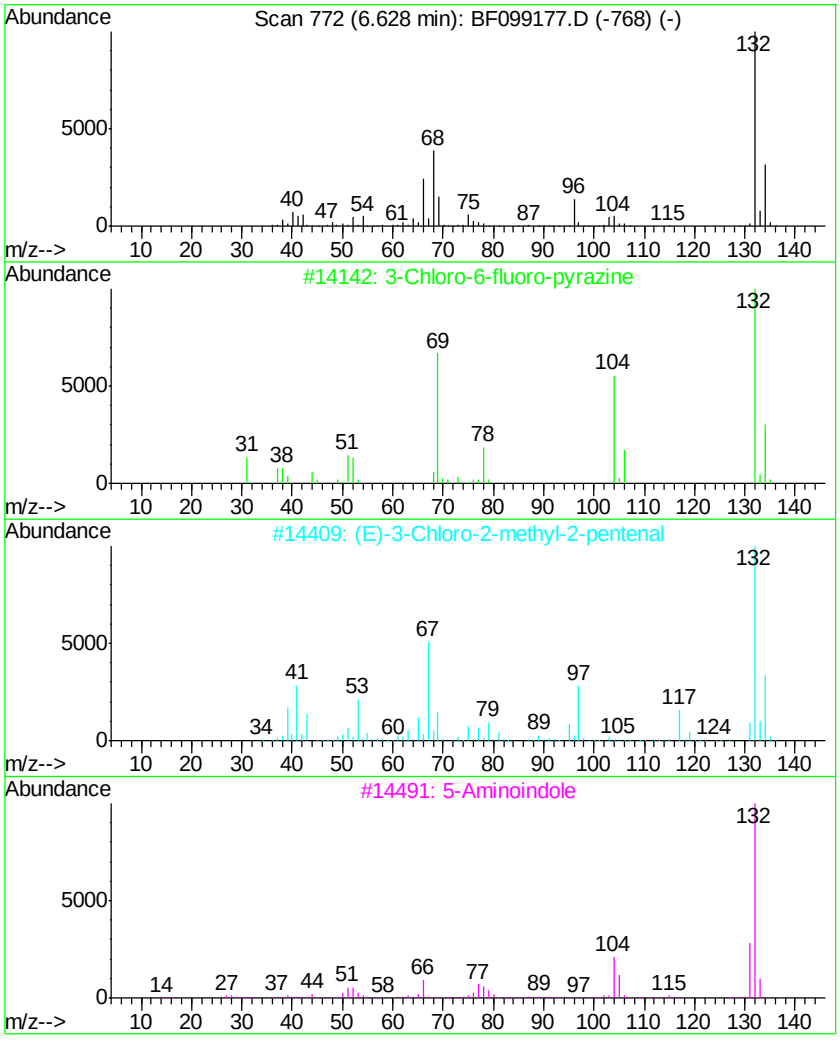
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

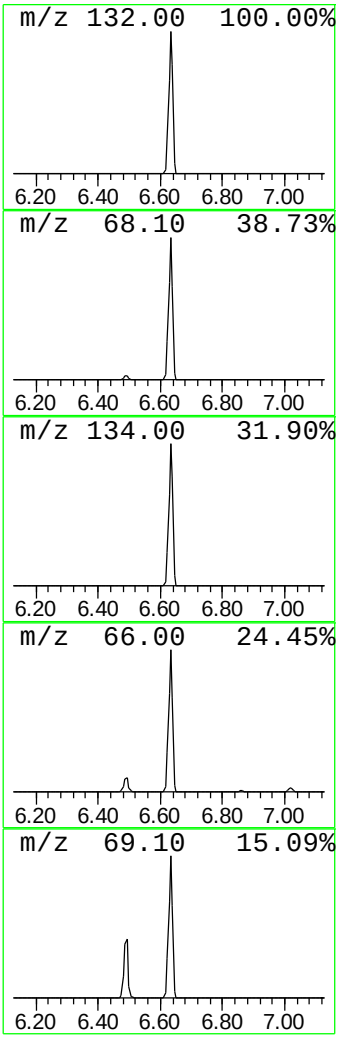
****

Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	77.69 ng	2958120	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	Xenon	132	Xe	007440-63-3	9





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Acq On : 7 Oct 2017 5:39
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Sample : I5542-07
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ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OWL-C8-GW

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

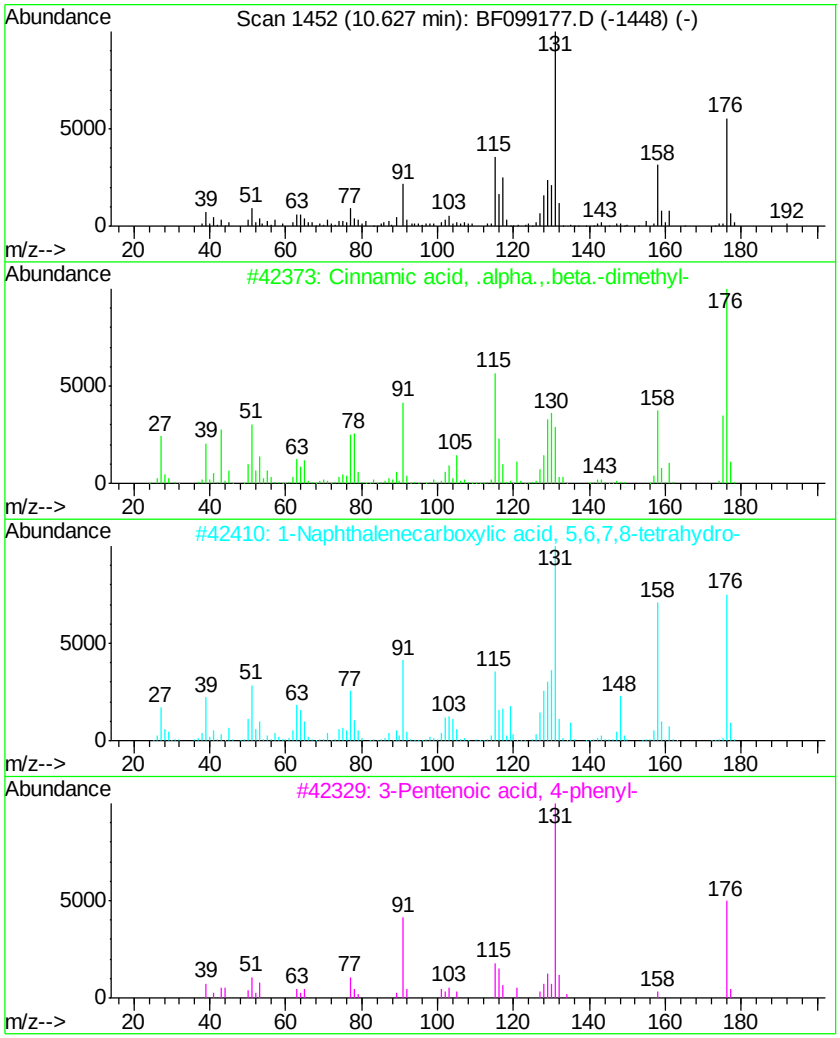
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

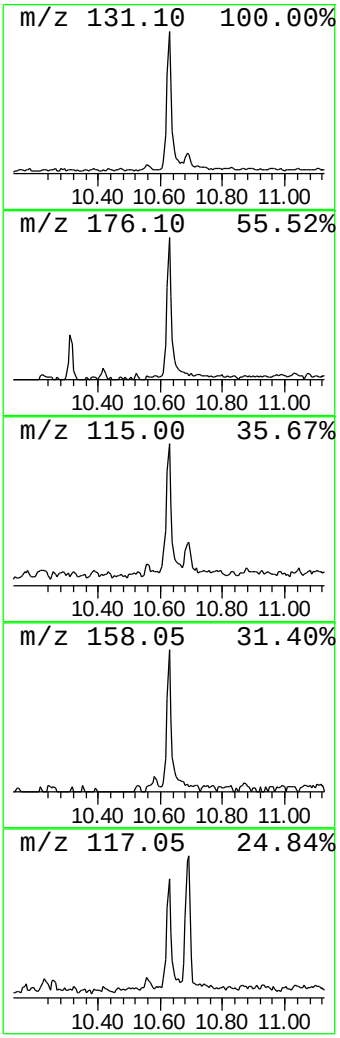
****

Peak Number 5 Cinnamic acid, .alpha.,.bet... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.63	3.40 ng	207251	Acenaphthene-d10	9.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamic acid, .alpha.,.beta.-di...	176	C11H12O2	1000151-56-4	60
2	1-Naphthalenecarboxylic acid, 5,...	176	C11H12O2	004242-18-6	59
3	3-Pentenoic acid, 4-phenyl-	176	C11H12O2	053774-19-9	58
4	1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	47
5	Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	43





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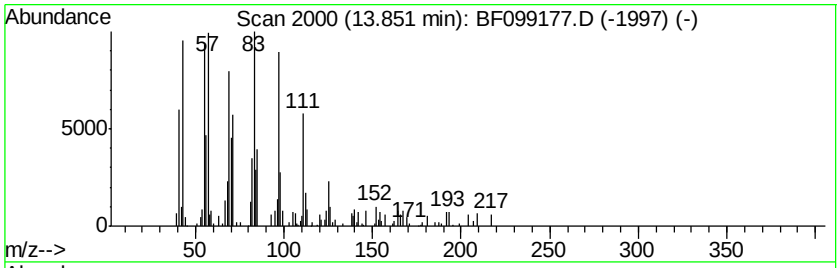
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

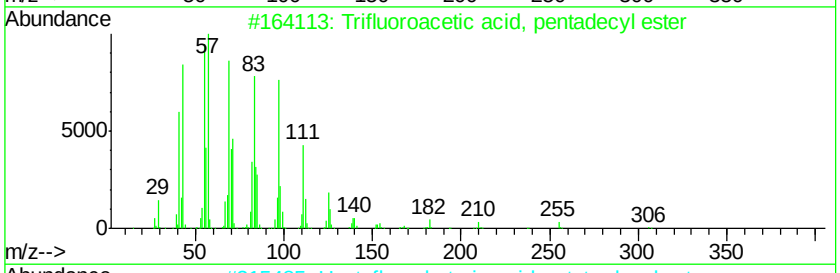
****

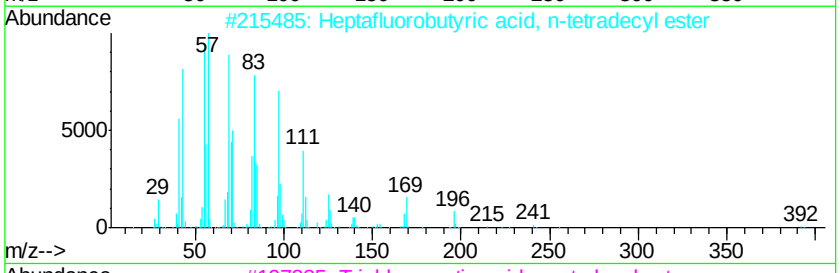
Peak Number 6 Trifluoroacetic acid, penta... Concentration Rank 7

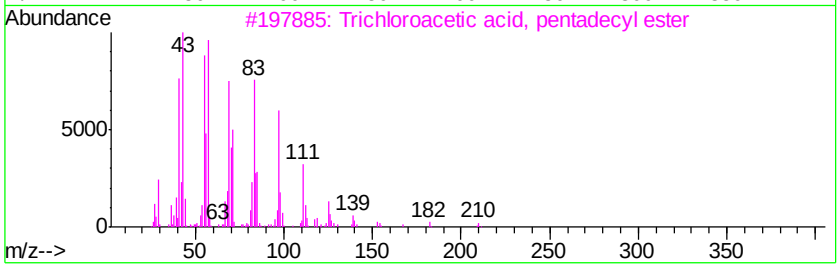
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	2.28 ng	73603	Chrysene-d12	14.02

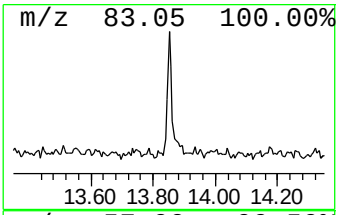
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
2	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	93
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4	11-Tricosene	322	C23H46	052078-56-5	91
5	1-Nonadecene	266	C19H38	018435-45-5	91

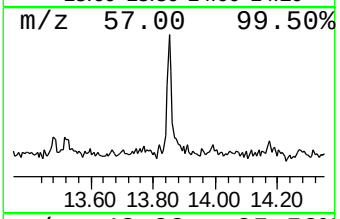


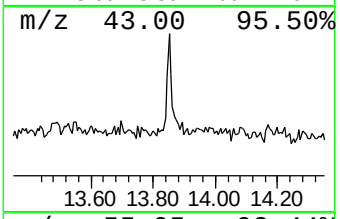


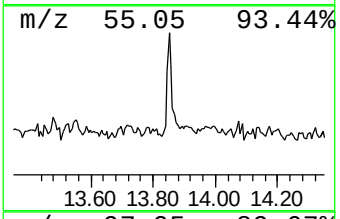


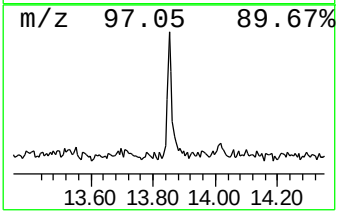












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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

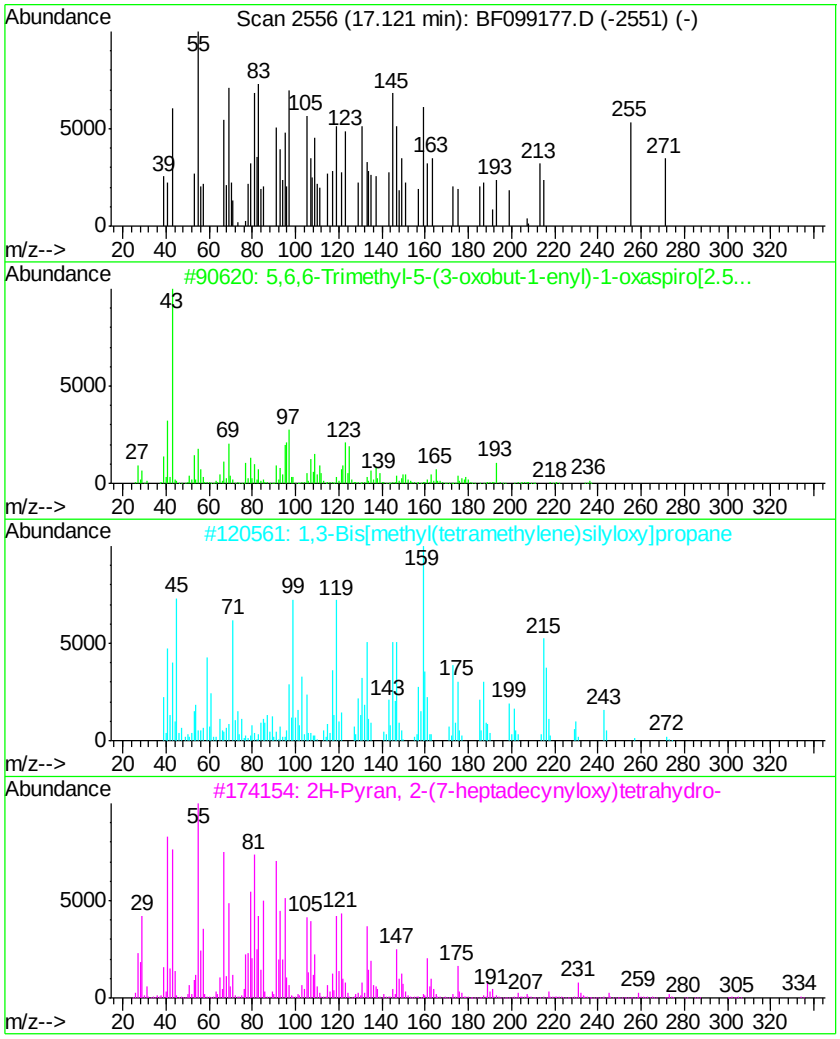
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

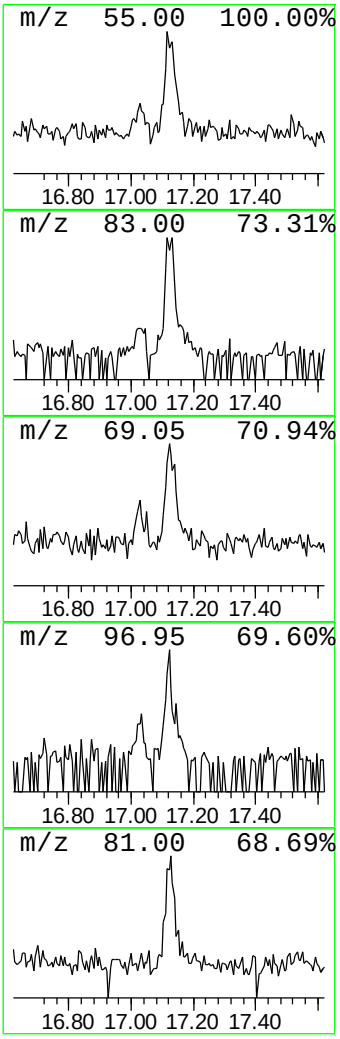
****

Peak Number 7 unknown17.12 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.12	2.36 ng	75109	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,6,6-Trimethyl-5-(3-oxobut-1-en...	236	C14H20O3	1000192-73-9	27
2	1,3-Bis[methyl(tetramethylene)si...	272	C13H28O2Si2	1000216-99-6	14
3	2H-Pyran, 2-(7-heptadecynyloxy)t...	336	C22H40O2	056599-50-9	14
4	9,12,15-Octadecatrienoic acid, 2...	436	C25H40O6	055320-01-9	12
5	9,12,15-Octadecatrienoic acid, 2...	436	C25H40O6	055320-02-0	12





Tentatively Identified Compound (LSC) summary

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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	20.9	ng	793939	1	6.86	761477	20.0
2-Pentanone, 4-hy...	5.09	7.2	ng	274954	1	6.86	761477	20.0
unknown6.63	6.63	77.7	ng	2958120	1	6.86	761477	20.0
Cinnamic acid, .a...	10.63	3.4	ng	207251	3	9.90	1218920	20.0
Trifluoroacetic a...	13.85	2.3	ng	73603	5	14.02	644476	20.0
unknown17.12	17.12	2.4	ng	75109	6	15.49	637743	20.0