LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100617\
Data File : BF099154.D
Acq On : 6 Oct 2017 18:24
Operator : SJ/JU
Sample : I5571-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PAMT-COMP-C

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	2.128	3	7	41	rVB	424702	647490	56.13%	6.205%
2	5.075	505	508	518	rVB	81006	82272	7.13%	0.788%
3	5.475	573	576	584	rVB	187159	158252	13.72%	1.517%
4	6.481	744	747	759	rVB2	145490	159390	13.82%	1.527%
5	6.628	769	772	775	rBV	306026	232914	20.19%	2.232%
6	6.863	808	812	815	rBV	975110	798201	69.20%	7.649%
7	7.016	834	838	842	rBV	761278	606076	52.54%	5.808%
8	7.422	903	907	910	rBV	615600	502199	43.54%	4.813%
9	7.504	917	921	929	rVB2	13943	17896	1.55%	0.171%
10	8.145	1025	1030	1033	rBV	1287707	1086929	94.23%	10.416%
11	9.216	1208	1212	1215	rBV	1227640	917513	79.54%	8.793%
12	9.610	1275	1279	1282	rBV	244949	193798	16.80%	1.857%
13	9.822	1308	1315	1317	rBV	56717	48037	4.16%	0.460%
14	9.898	1324	1328	1336	rBV	1360669	1153496	100.00%	11.054%
15	10.057	1349	1355	1357	rBV2	8681	13818	1.20%	0.132%
16	10.316	1392	1399	1403	rBV2	83013	88925	7.71%	0.852%
17	10.539	1432	1437	1439	rBV2	20081	26730	2.32%	0.256%
18	10.563	1439	1441	1444	rVB	67958	58486	5.07%	0.560%
19	10.686	1459	1462	1470	rVB	140881	139272	12.07%	1.335%
20	10.792	1477	1480	1489	rBV	92798	92809	8.05%	0.889%
21	10.986	1510	1513	1517	rBV3	8684	13034	1.13%	0.125%
22	11.239	1553	1556	1558	rBV	44655	33581	2.91%	0.322%
23	11.269	1558	1561	1567	rVB3	11897	14419	1.25%	0.138%
24	11.386	1577	1581	1584	rBV	1333325	1130608	98.02%	10.835%
25	12.474	1761	1766	1769	rBV2	13670	15027	1.30%	0.144%
26	12.963	1845	1849	1852	rBV	768648	619134	53.67%	5.933%
27	13.851	1996	2000	2014	rBV2	94444	117330	10.17%	1.124%
28	13.992	2018	2024	2026	rBV	14345	14731	1.28%	0.141%
29	14.021	2026	2029	2033	rBV	897594	769507	66.71%	7.374%
30	14.857	2168	2171	2174	rBV2	14929	14058	1.22%	0.135%
31	15.492	2273	2279	2289	rBV	471160	618916	53.66%	5.931%
32	15.933	2349	2354	2360	rBV3	11883	18075	1.57%	0.173%
33	16.439	2436	2440	2445	rBV4	9056	16085	1.39%	0.154%
34	17.733	2654	2660	2667	rVB9	6797	16035	1.39%	0.154%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100617\
Data File : BF099154.D
Acq On : 6 Oct 2017 18:24
Operator : SJ/JU
Sample : I5571-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PAMT-COMP-C

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

Sum of corrected areas: 10435043

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100617\
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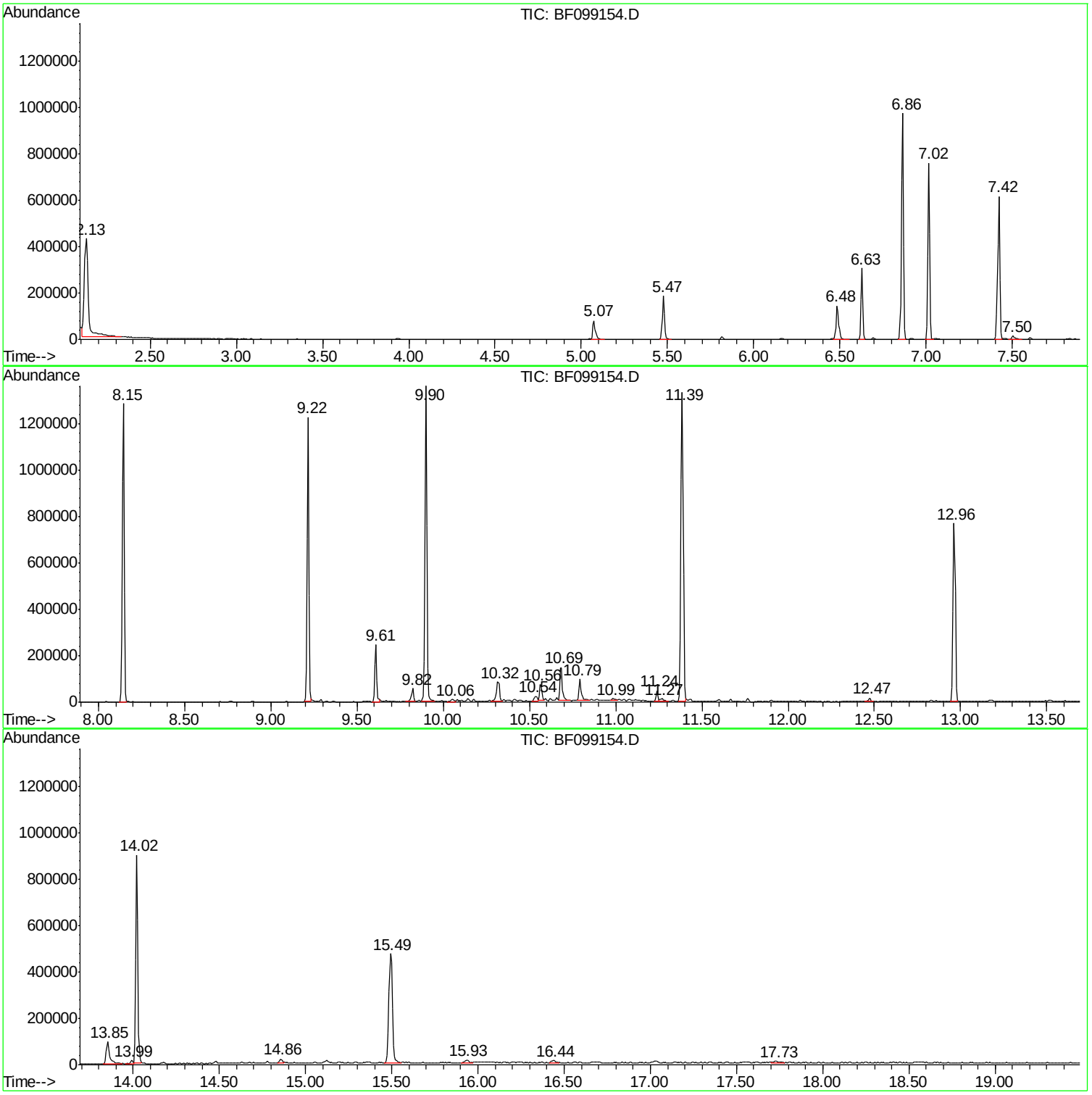
Acq On : 6 Oct 2017 18:24
Operator : SJ/JU
Sample : I5571-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PAMT-COMP-C

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100617\
Data File : BF099154.D
Acq On : 6 Oct 2017 18:24
Operator : SJ/JU
Sample : I5571-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PAMT-COMP-C

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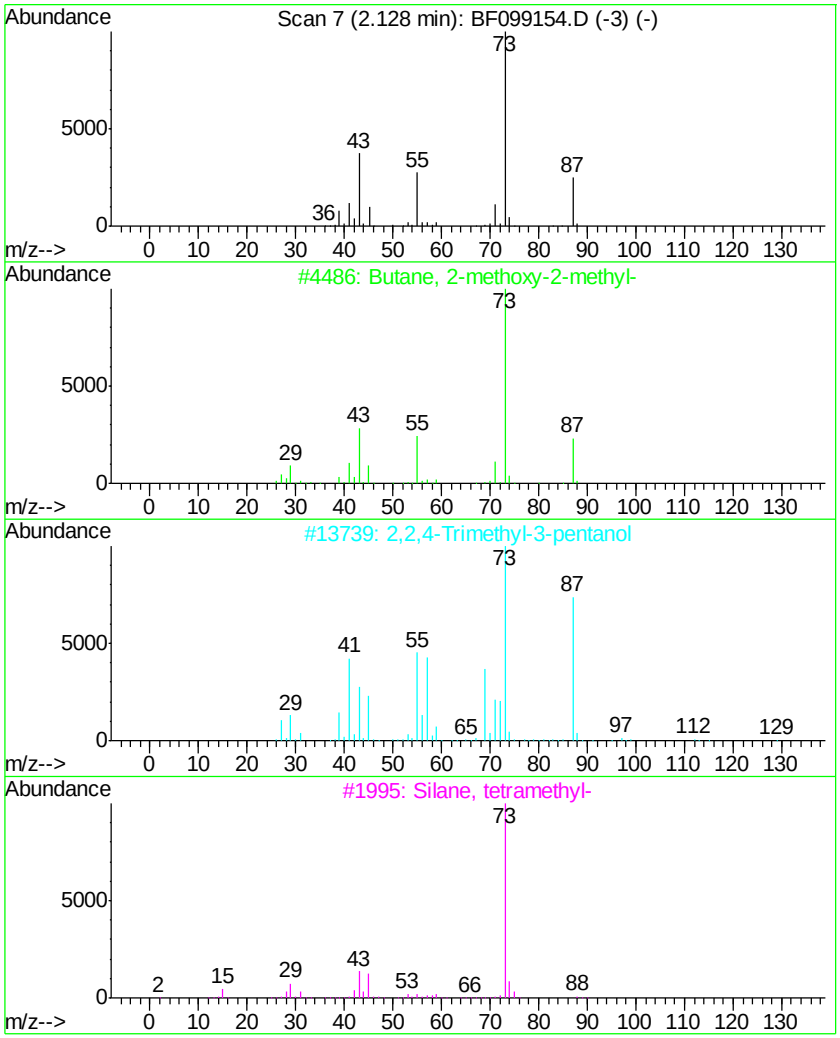
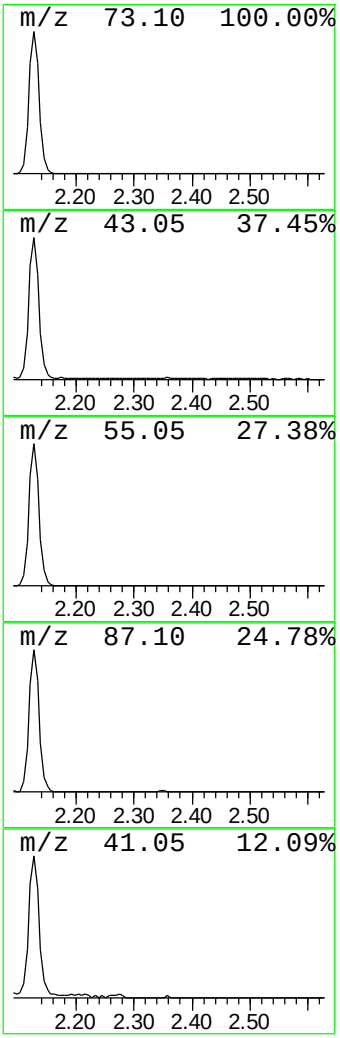
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	16.22 ng	647490	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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32
5	1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	23





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100617\
Data File : BF099154.D
Acq On : 6 Oct 2017 18:24
Operator : SJ/JU
Sample : I5571-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PAMT-COMP-C

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

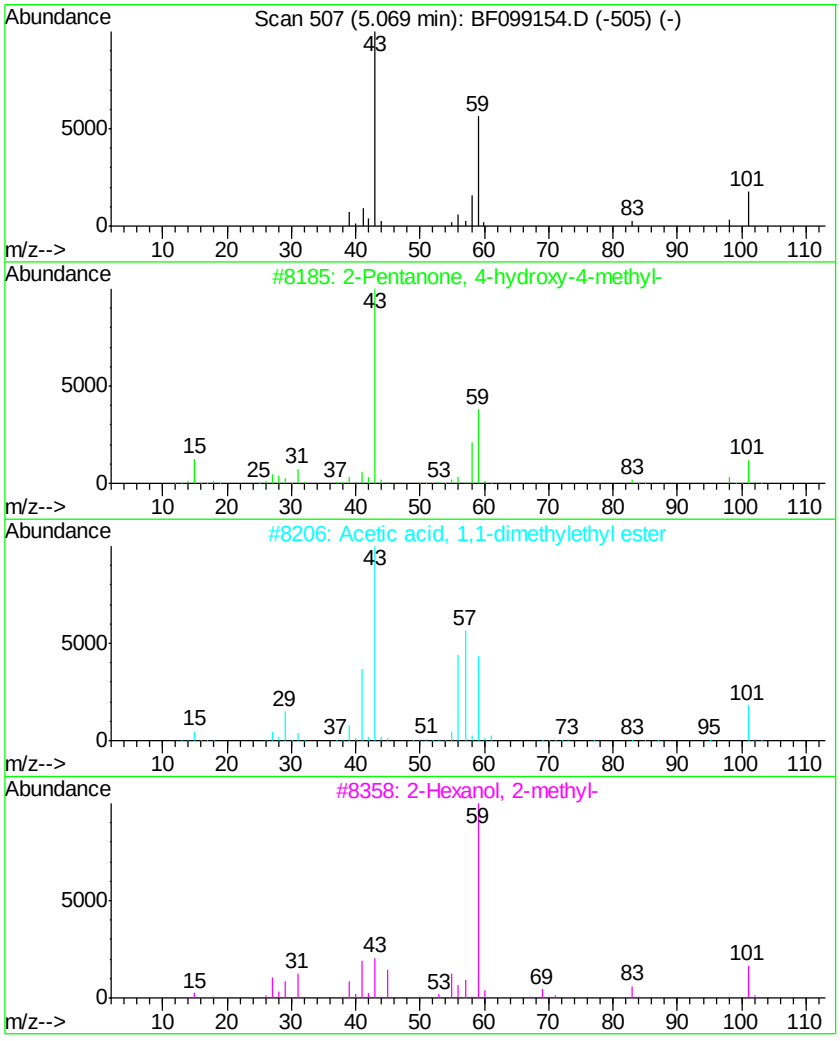
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

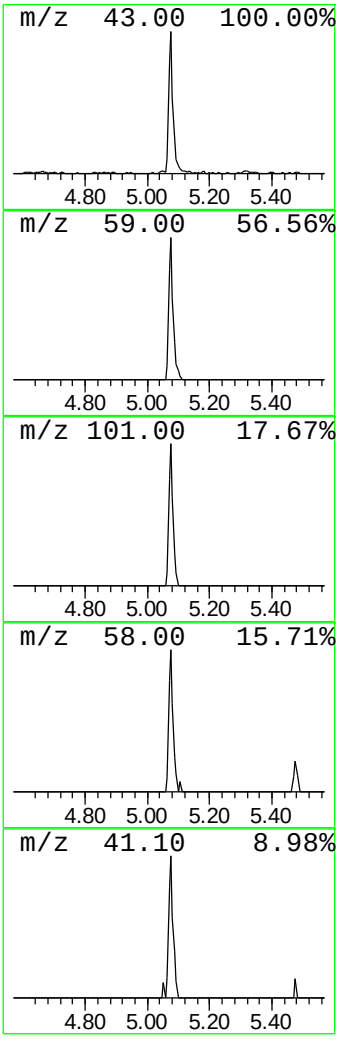
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	2.06 ng	82272	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	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Sample : I5571-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PAMT-COMP-C

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

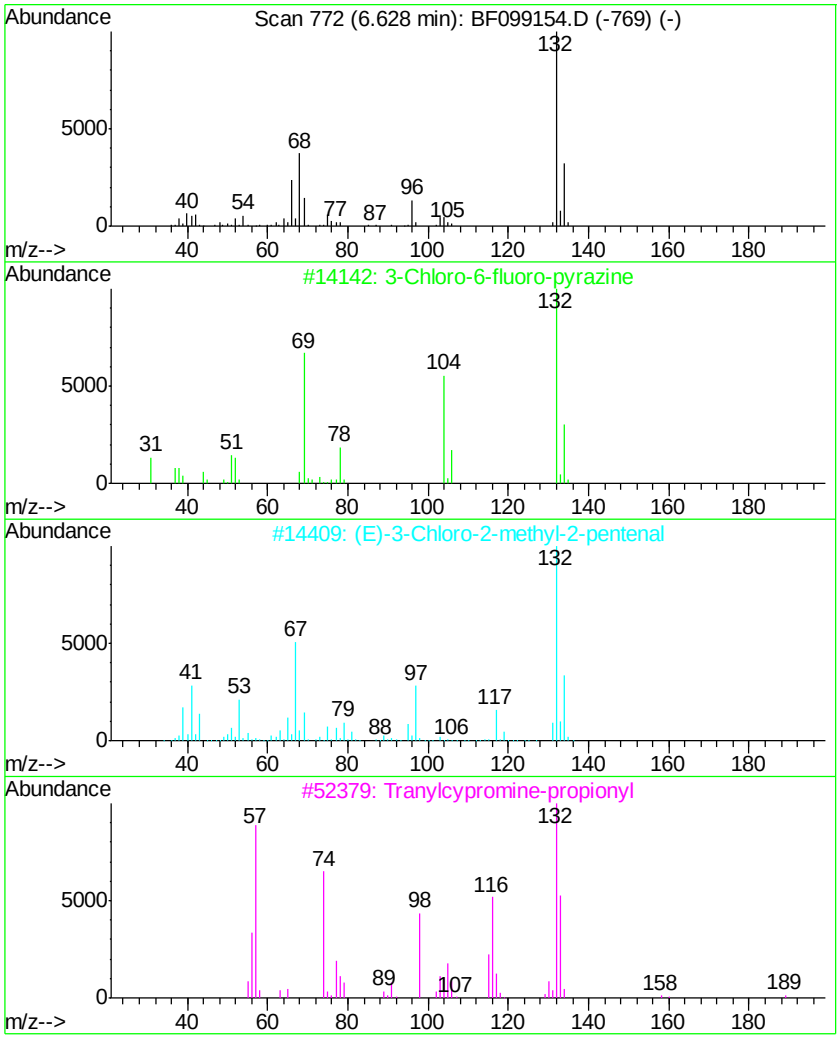
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

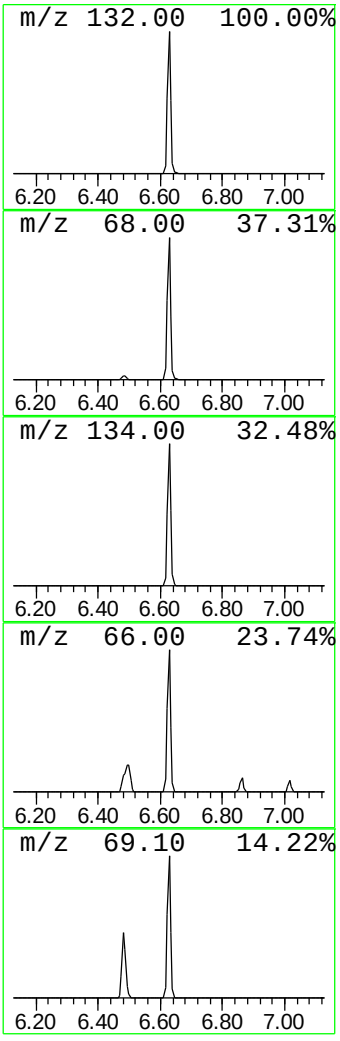
****

Peak Number 3 unknown6.63 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	5.84 ng	232914	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	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Amphetaminil	250	C17H18N2	017590-01-1	12
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Sample : I5571-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PAMT-COMP-C

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

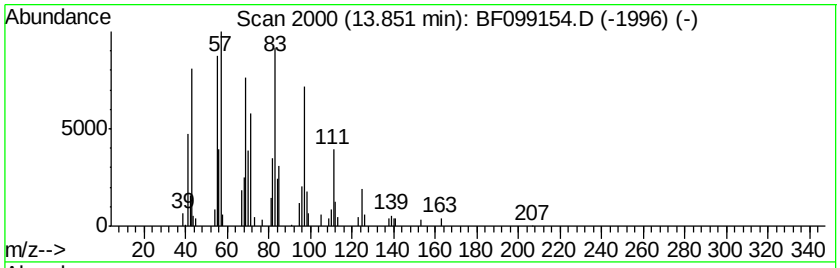
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

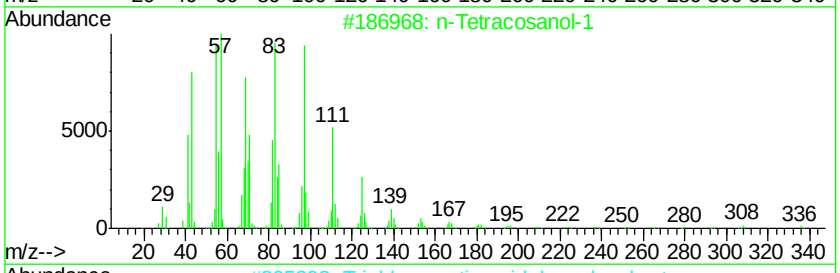
****

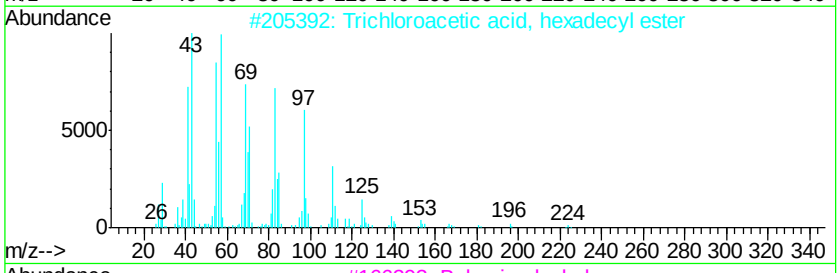
Peak Number 5 n-Tetracosanol-1 Concentration Rank 4

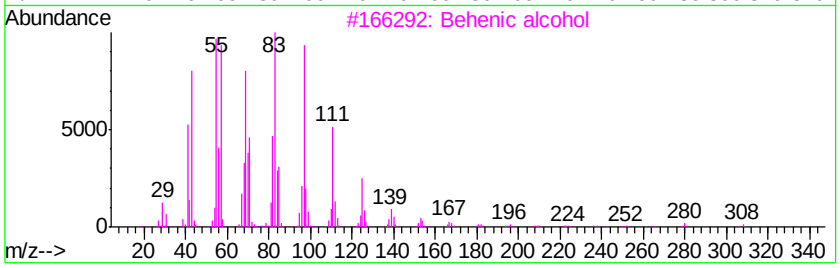
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	3.05 ng	117330	Chrysene-d12	14.02

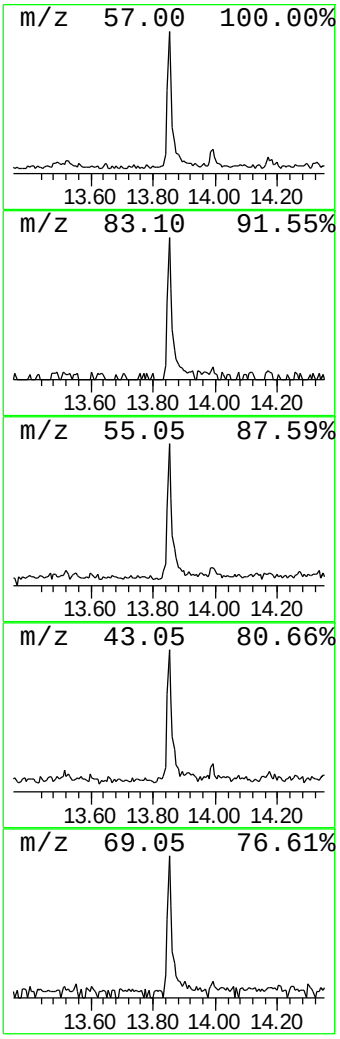
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	Behenic alcohol	326	C22H46O	000661-19-8	91
4	1-Hexacosanol	382	C26H54O	000506-52-5	91
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91











Tentatively Identified Compound (LSC) summary

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Instrument : BNA_F
ClientSampleId : PAMT-COMP-C

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...	2.13	16.2	ng	647490	1	6.86	798201	20.0
2-Pentanone, 4-hy...	5.07	2.1	ng	82272	1	6.86	798201	20.0
unknown6.63	6.63	5.8	ng	232914	1	6.86	798201	20.0
n-Tetracosanol-1	13.85	3.0	ng	117330	5	14.02	769507	20.0