LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092615\
Data File : BF081828.D
Acq On : 26 Sep 2015 15:24
Operator : UM/IZ
Sample : G3754-07
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-9B

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-BF092415.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	2.937	67	70	74	rVB	30582	47435	1.37%	0.191%
2	3.577	123	126	130	rVB	54740	87956	2.54%	0.355%
3	4.503	203	207	209	rBV	1674760	2219813	64.22%	8.948%
4	4.766	228	230	233	rBV	74947	88294	2.55%	0.356%
5	5.131	260	262	264	rVB	278750	376006	10.88%	1.516%
6	5.531	294	297	299	rBV	1469463	1295305	37.47%	5.221%
7	6.549	384	386	389	rBV	1169643	1058368	30.62%	4.266%
8	6.697	397	399	402	rBV	1671449	1503123	43.48%	6.059%
9	6.937	418	420	422	rBV	913261	743735	21.51%	2.998%
10	7.097	431	434	436	rVB	2248434	2375790	68.73%	9.577%
11	7.497	466	469	471	rBV	1307420	1858323	53.76%	7.491%
12	7.532	471	472	474	rVB	119850	85520	2.47%	0.345%
13	8.229	530	533	535	rBV	695300	906717	26.23%	3.655%
14	9.303	624	627	629	rBV	3739156	3456841	100.00%	13.934%
15	9.692	659	661	663	rBV	302005	241254	6.98%	0.972%
16	9.978	684	686	689	rBV	1057135	1032017	29.85%	4.160%
17	10.766	752	755	758	rBV	1380207	1251842	36.21%	5.046%
18	11.464	814	816	819	rBV	1040315	1045981	30.26%	4.216%
19	12.618	915	917	919	rBV	61221	49801	1.44%	0.201%
20	13.052	953	955	958	rBV	2457509	3328512	96.29%	13.417%
21	13.944	1031	1033	1041	rVB2	72613	90672	2.62%	0.365%
22	14.104	1045	1047	1050	rVB	812260	873754	25.28%	3.522%
23	14.812	1107	1109	1111	rVB	38249	37430	1.08%	0.151%
24	15.452	1161	1165	1169	rBV3	35442	66704	1.93%	0.269%
25	15.578	1173	1176	1179	rBV	495356	621411	17.98%	2.505%
26	21.465	1686	1691	1698	rVB3	17026	65423	1.89%	0.264%

Sum of corrected areas: 24808027

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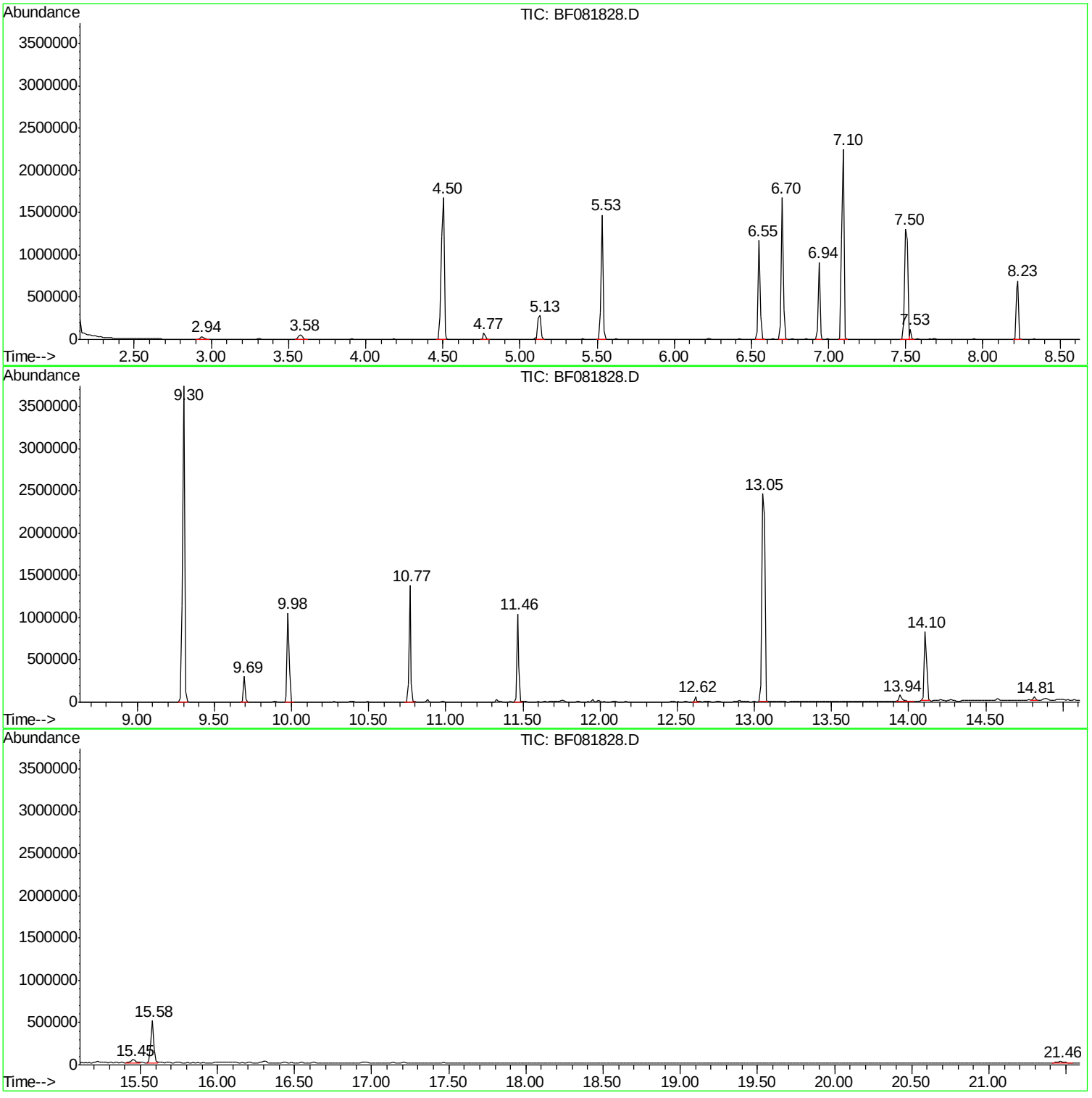
Instrument :
BNA_F
ClientSampleId :
MW-9B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.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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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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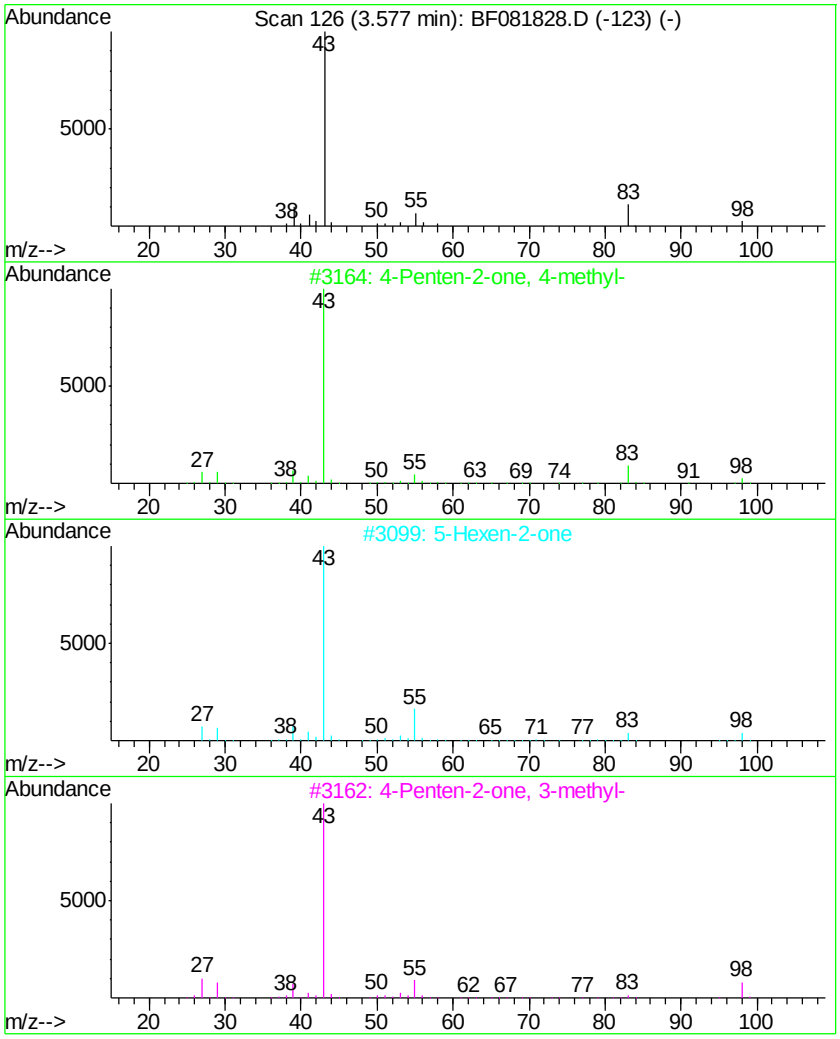
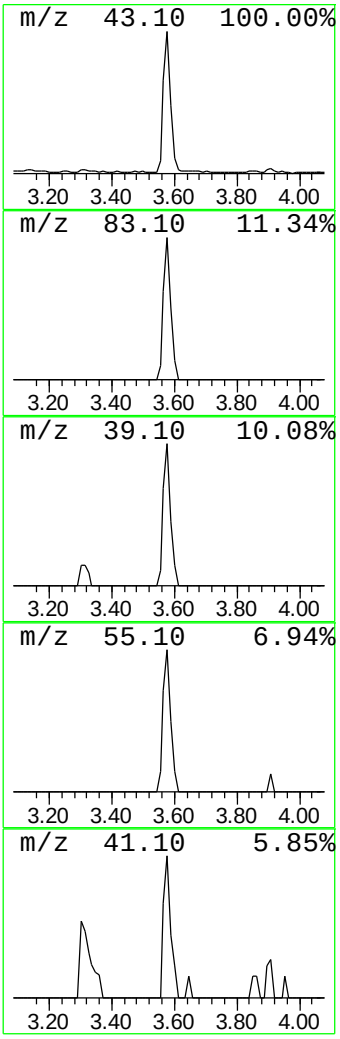
Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.58	2.37 ng	87956	1,4-Dichlorobenzene-d4	6.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	86
2	5-Hexen-2-one	98	C6H10O	000109-49-9	52
3	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	28
4	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	9
5	4-Hexen-2-one	98	C6H10O	025659-22-7	9





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Acq On : 26 Sep 2015 15:24
Operator : UM/IZ
Sample : G3754-07
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-9B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.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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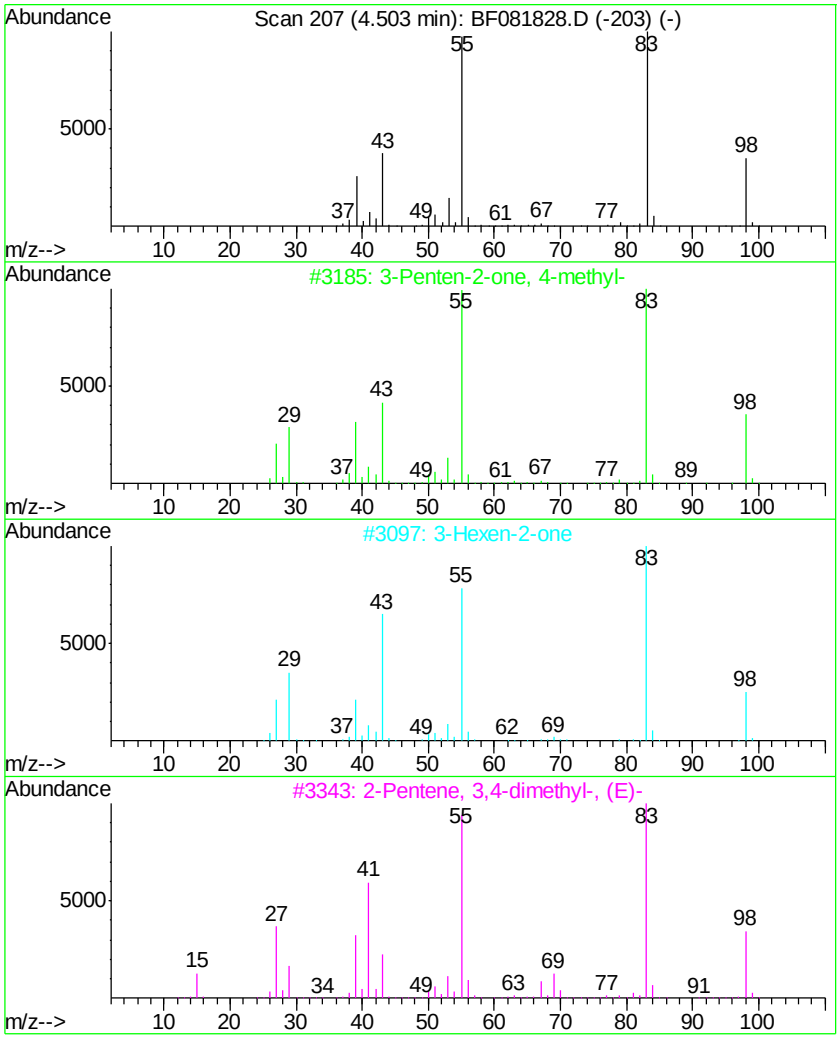
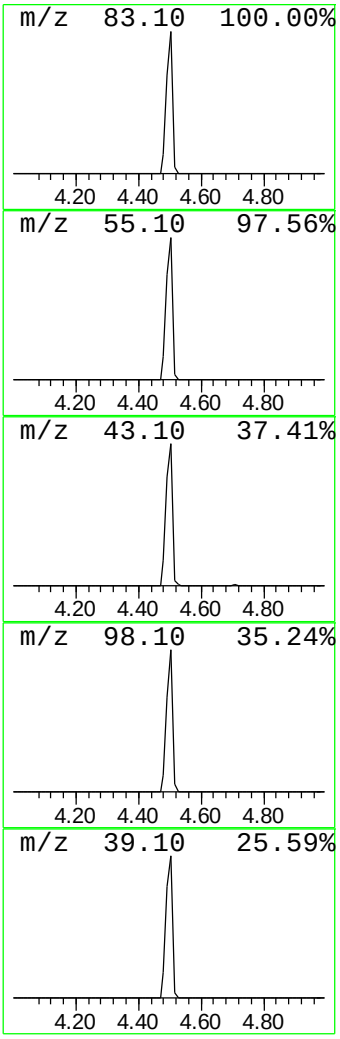
Peak Number 2 3-Hexen-2-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.50	59.69 ng	2219810	1,4-Dichlorobenzene-d4	6.94

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	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





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Data File : BF081828.D
Acq On : 26 Sep 2015 15:24
Operator : UM/IZ
Sample : G3754-07
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-9B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.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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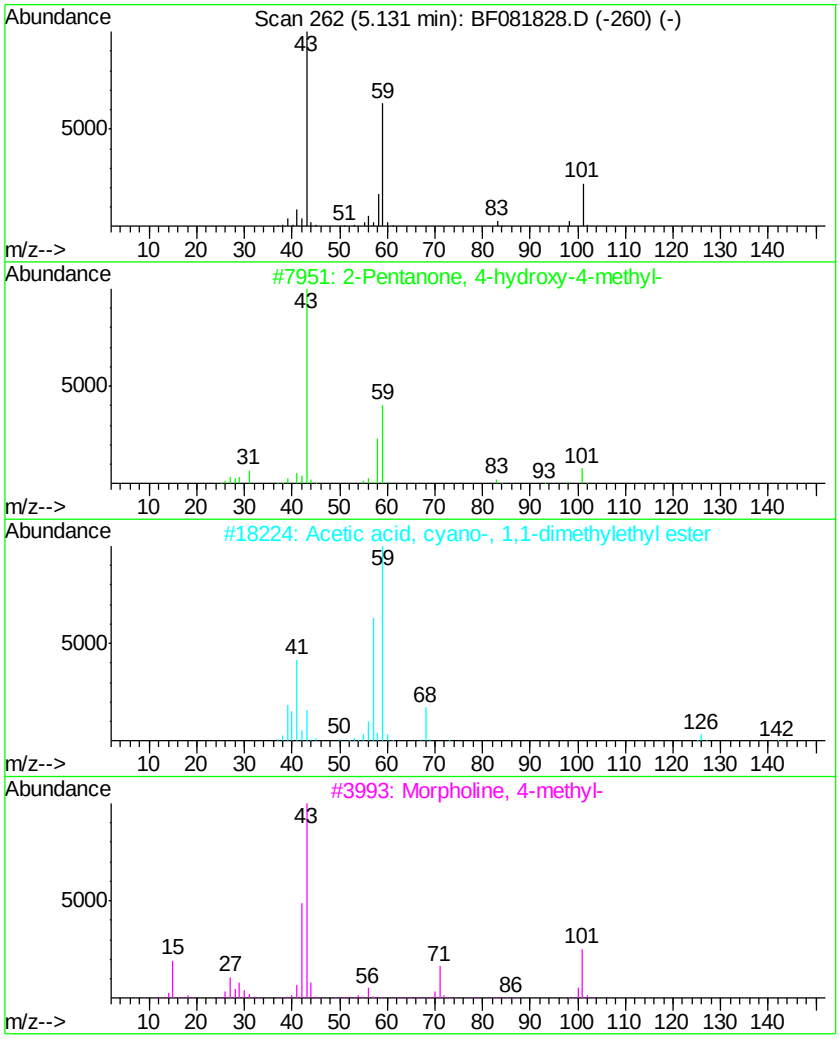
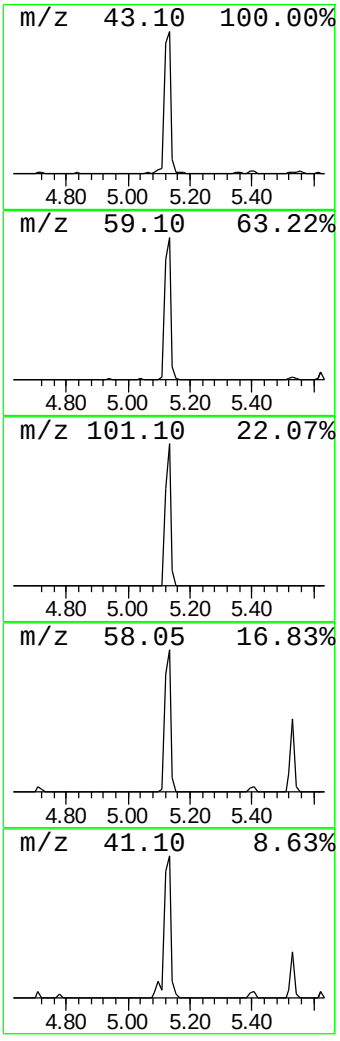
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	10.11 ng	376006	1,4-Dichlorobenzene-d4	6.94

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	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Guanidine	59	CH5N3	000113-00-8	9





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Misc :
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Instrument : BNA_F
ClientSampleId : MW-9B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.M
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TIC Library : C:\DATABASE\NIST02.L
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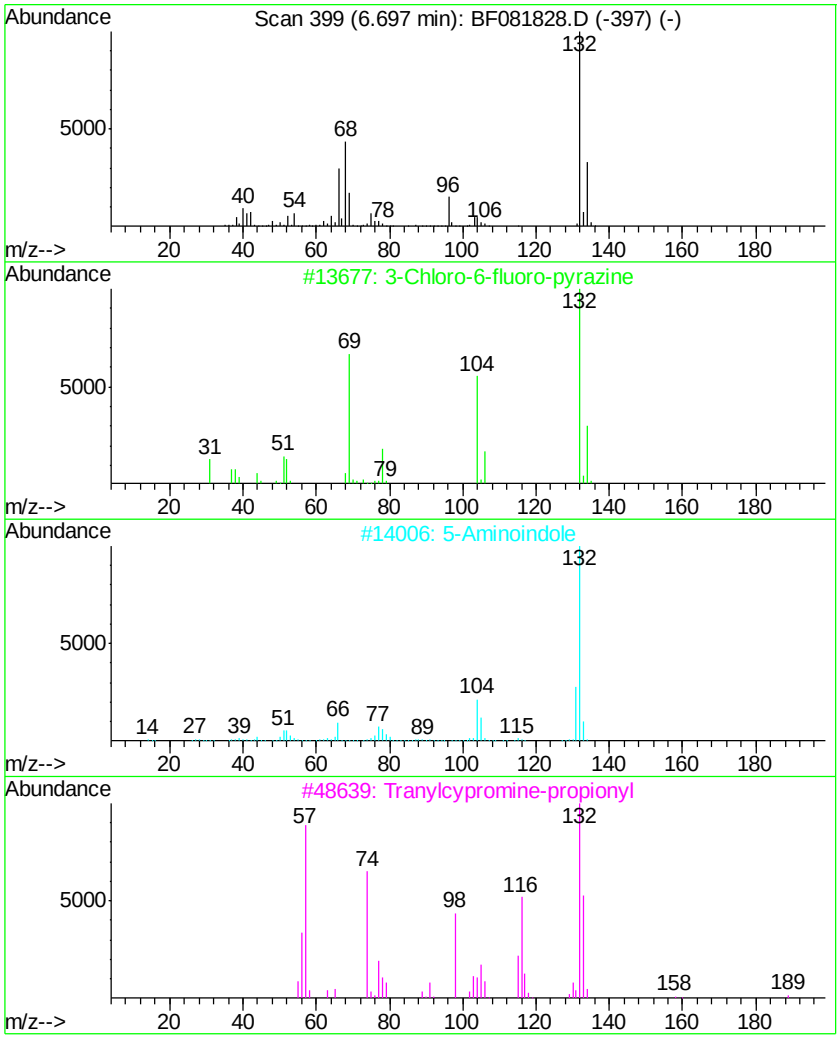
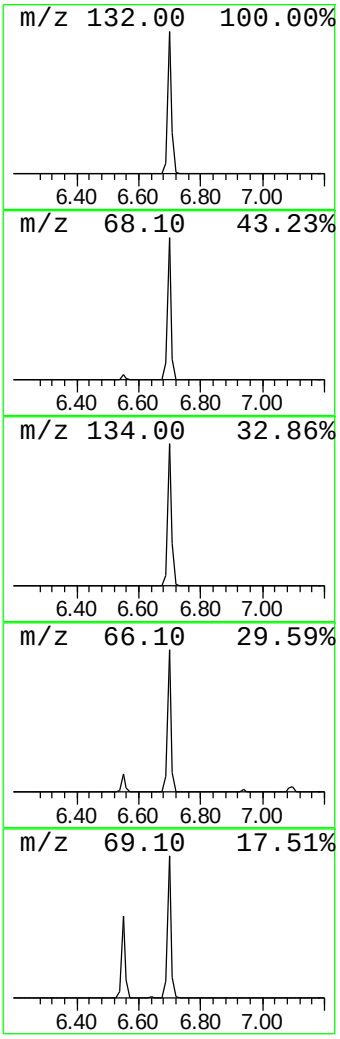
Peak Number 5 unknown6.70 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	40.42 ng	1503120	1,4-Dichlorobenzene-d4	6.94

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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





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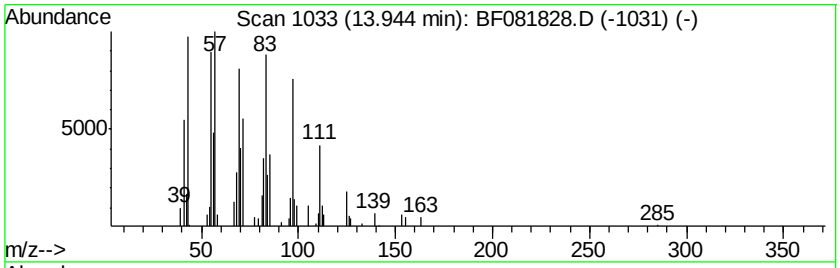
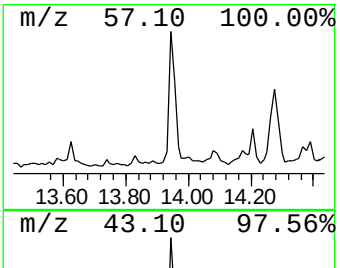
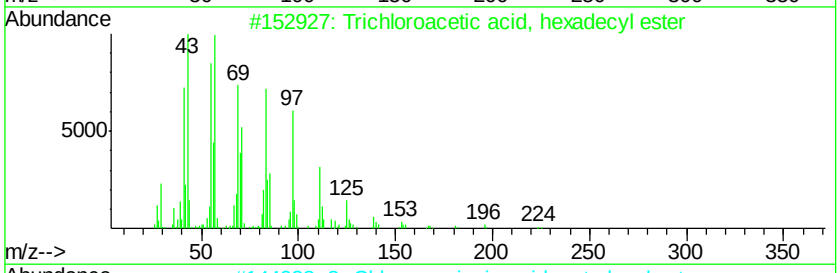
Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 9

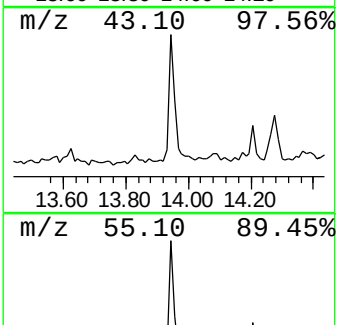
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	2.08 ng	90672	Chrysene-d12	14.10

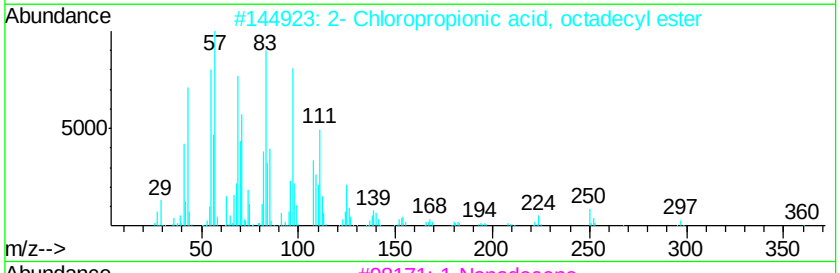
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	1-Tetracosanol	354	C24H50O	000506-51-4	91
5	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91

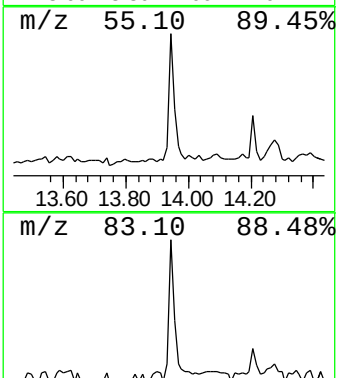


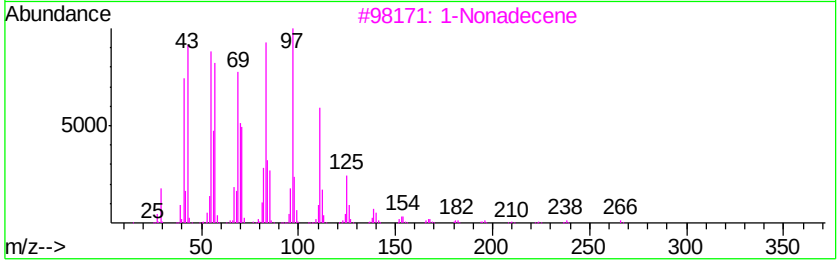


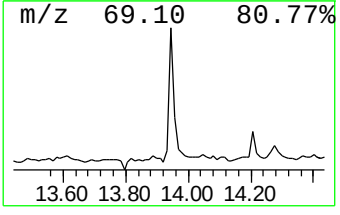












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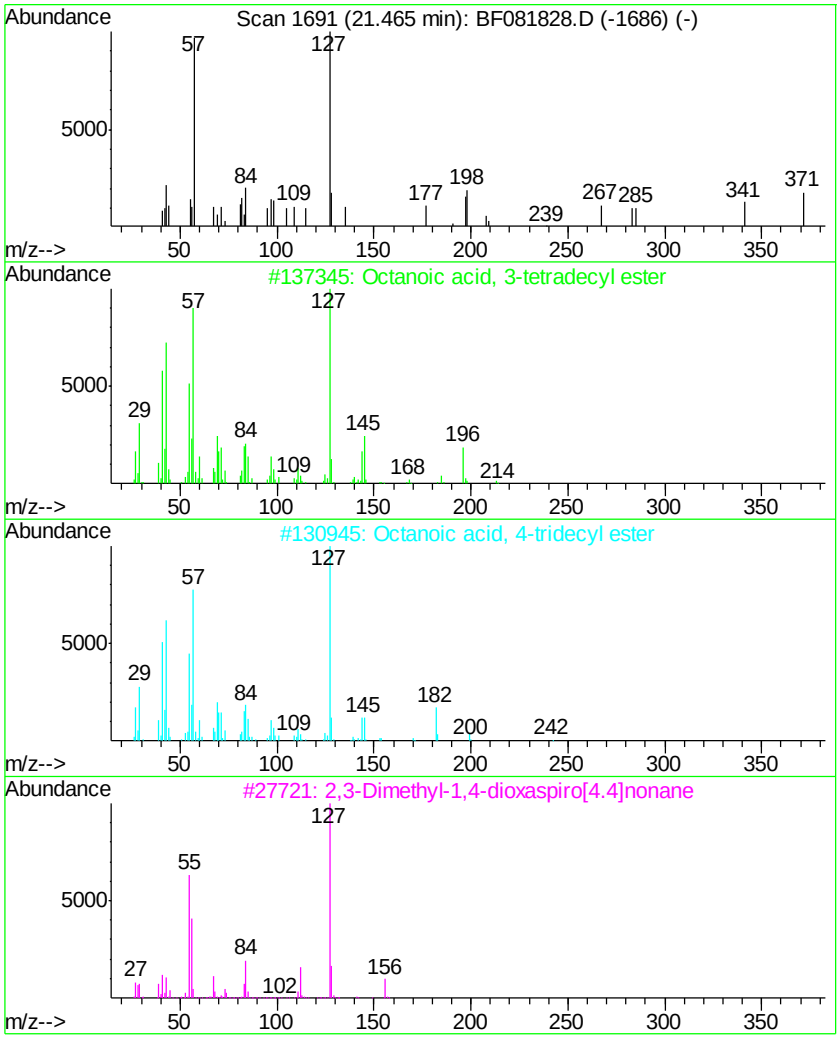
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

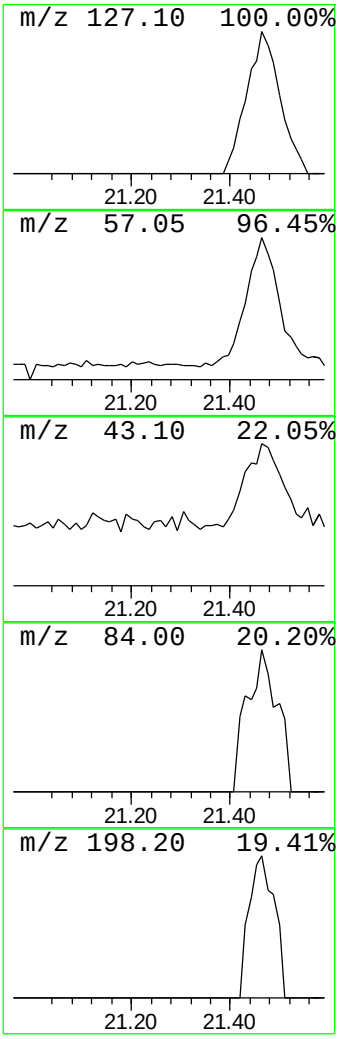
****

Peak Number 9 unknown21.46 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.46	2.11 ng	65423	Perylene-d12	15.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid, 3-tetradecyl ester	340	C22H44O2	1000280-62-8	37
2	Octanoic acid, 4-tridecyl ester	326	C21H42O2	1000280-62-6	37
3	2,3-Dimethyl-1,4-dioxaspiro[4.4]...	156	C9H16O2	006290-15-9	35
4	1,4-Dioxaspiro[4,5]decane-7-buta...	284	C16H28O4	1000195-79-0	27
5	Propylphosphonic acid, fluoroanh...	224	C10H22FO2P	333416-19-6	27





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
4-Penten-2-one, 4...	3.58	2.4	ng	87956	1	6.94	743735	20.0
3-Hexen-2-one	4.50	59.7	ng	2219810	1	6.94	743735	20.0
2-Pentanone, 4-hy...	5.13	10.1	ng	376006	1	6.94	743735	20.0
unknown6.70	6.70	40.4	ng	1503120	1	6.94	743735	20.0
Trichloroacetic a...	13.94	2.1	ng	90672	5	14.10	873754	20.0
unknown21.46	21.46	2.1	ng	65423	6	15.58	621411	20.0