LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093645.D
Acq On : 14 Mar 2017 8:57
Operator : SJ/MA
Sample : I2201-21
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-121

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-BF030717.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	2.435	46	48	64	rVB	80807	223826	4.04%	0.466%
2	3.121	106	108	125	rBV	163479	455665	8.23%	0.949%
3	4.173	197	200	218	rBV	1153813	2411799	43.55%	5.025%
4	4.401	218	220	223	rVV	61262	104406	1.89%	0.218%
5	4.458	223	225	228	rVB	62166	85365	1.54%	0.178%
6	4.881	260	262	277	rBV	635110	1370290	24.74%	2.855%
7	5.316	298	300	328	rBV	3692710	5538295	100.00%	11.540%
8	6.367	391	392	400	rBV	3143938	4988161	90.07%	10.394%
9	6.482	400	402	405	rVB	4578669	4809860	86.85%	10.022%
10	6.710	420	422	433	rVB	959630	1016343	18.35%	2.118%
11	6.859	433	435	438	rBV	3792147	3856472	69.63%	8.036%
12	7.282	470	472	487	rBV	2848135	3513116	63.43%	7.320%
13	8.002	533	535	549	rVB	1183382	1462005	26.40%	3.046%
14	9.076	627	629	632	rBV	4057588	5472335	98.81%	11.402%
15	9.762	686	689	691	rBV	1067585	1434541	25.90%	2.989%
16	10.551	756	758	761	rBV2	2227413	2917911	52.69%	6.080%
17	11.248	817	819	826	rBV	1481634	1478234	26.69%	3.080%
18	12.654	940	942	944	rVB	175605	143366	2.59%	0.299%
19	12.836	955	958	960	rBV	4605348	4908033	88.62%	10.227%
20	13.362	1001	1004	1006	rBV	81023	92663	1.67%	0.193%
21	13.899	1049	1051	1061	rBV	844196	1153715	20.83%	2.404%
22	15.305	1172	1174	1184	rVB	282887	556047	10.04%	1.159%

Sum of corrected areas: 47992448

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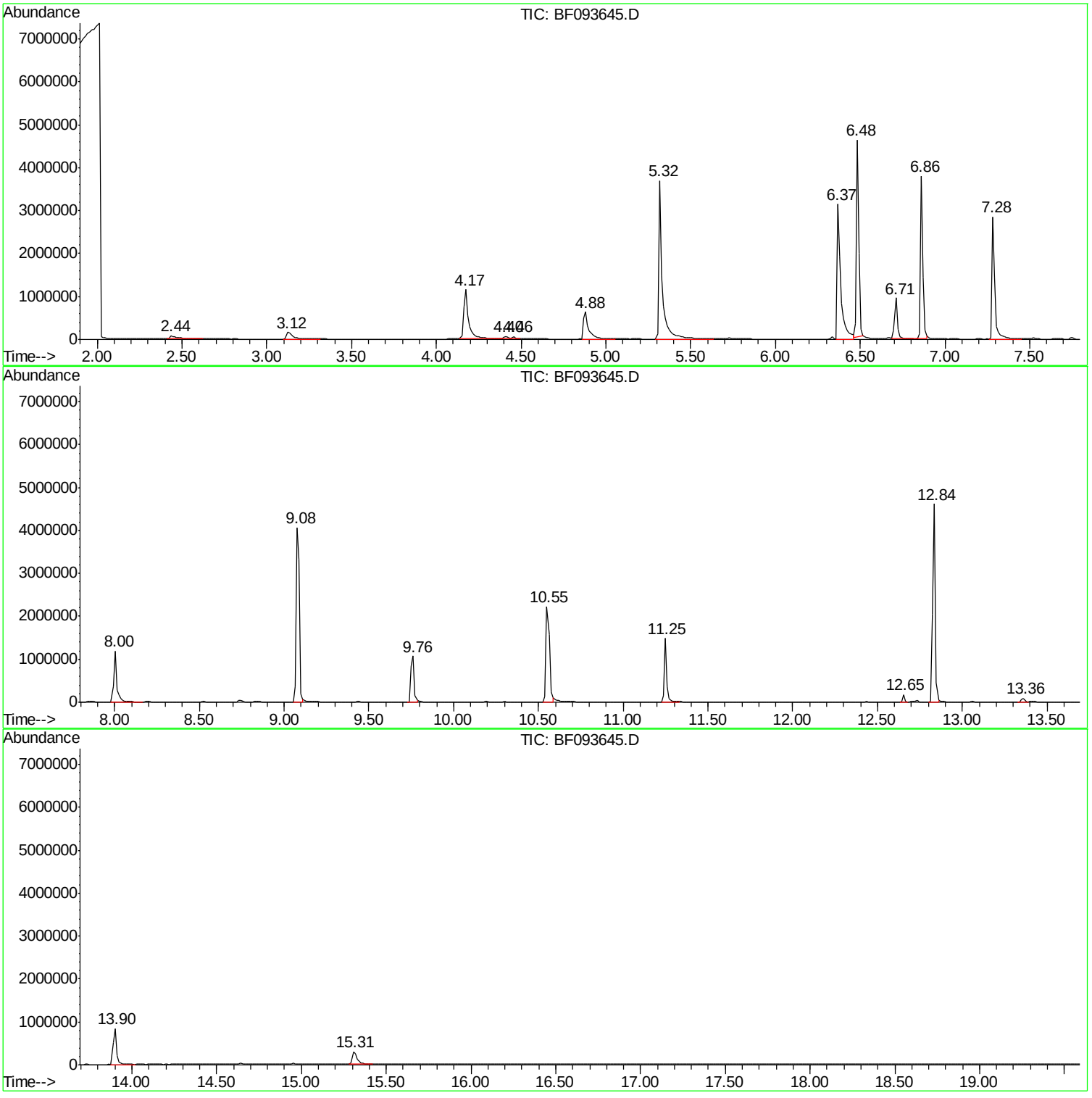
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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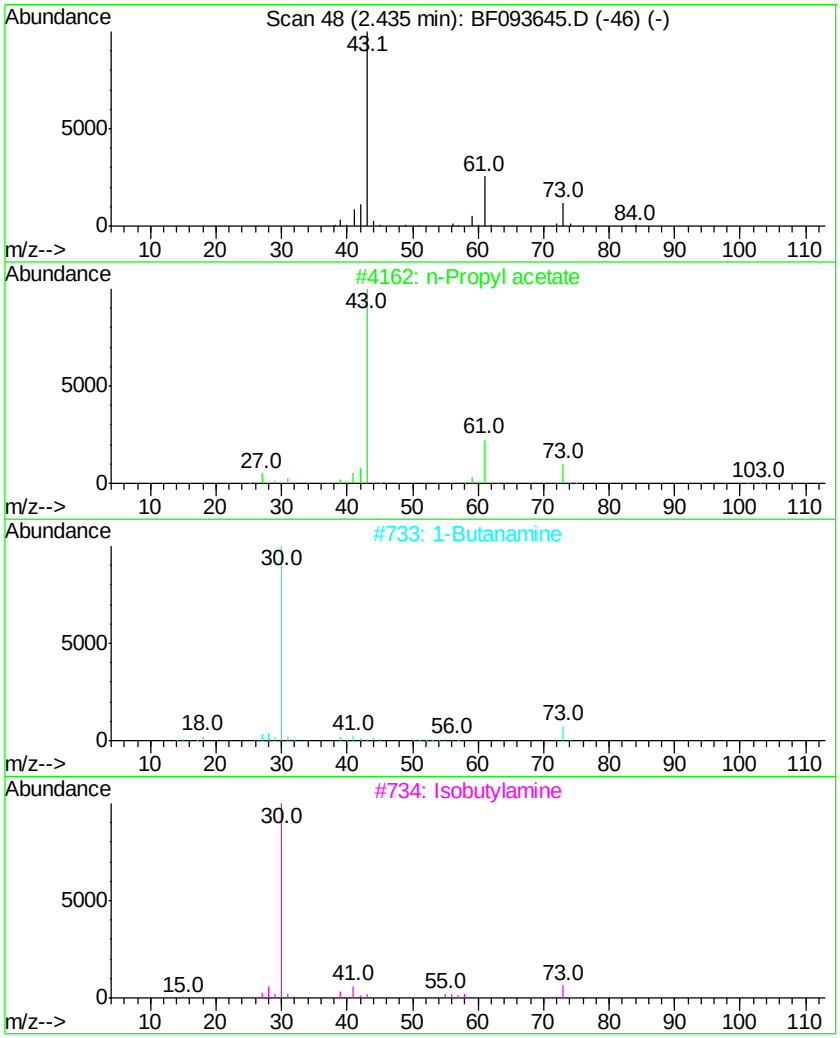
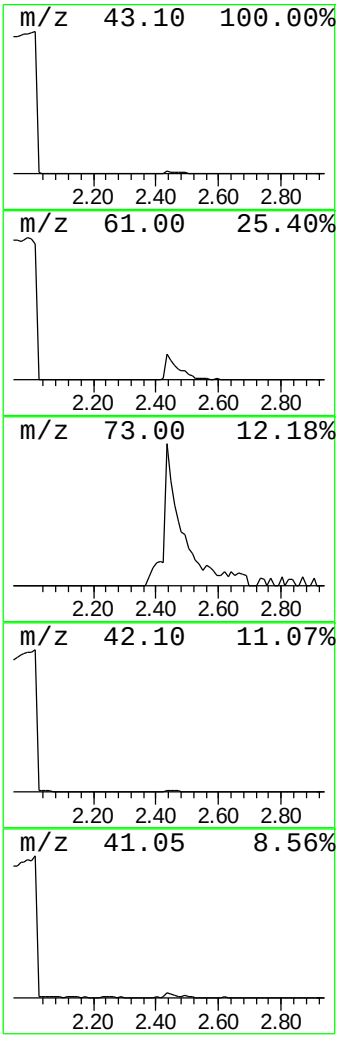
Peak Number 1 n-Propyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.44	4.40 ng	223826	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	78
2	1-Butanamine	73	C4H11N	000109-73-9	7
3	Isobutylamine	73	C4H11N	000078-81-9	5
4	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	4
5	Butane, 2-methyl-	72	C5H12	000078-78-4	4





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
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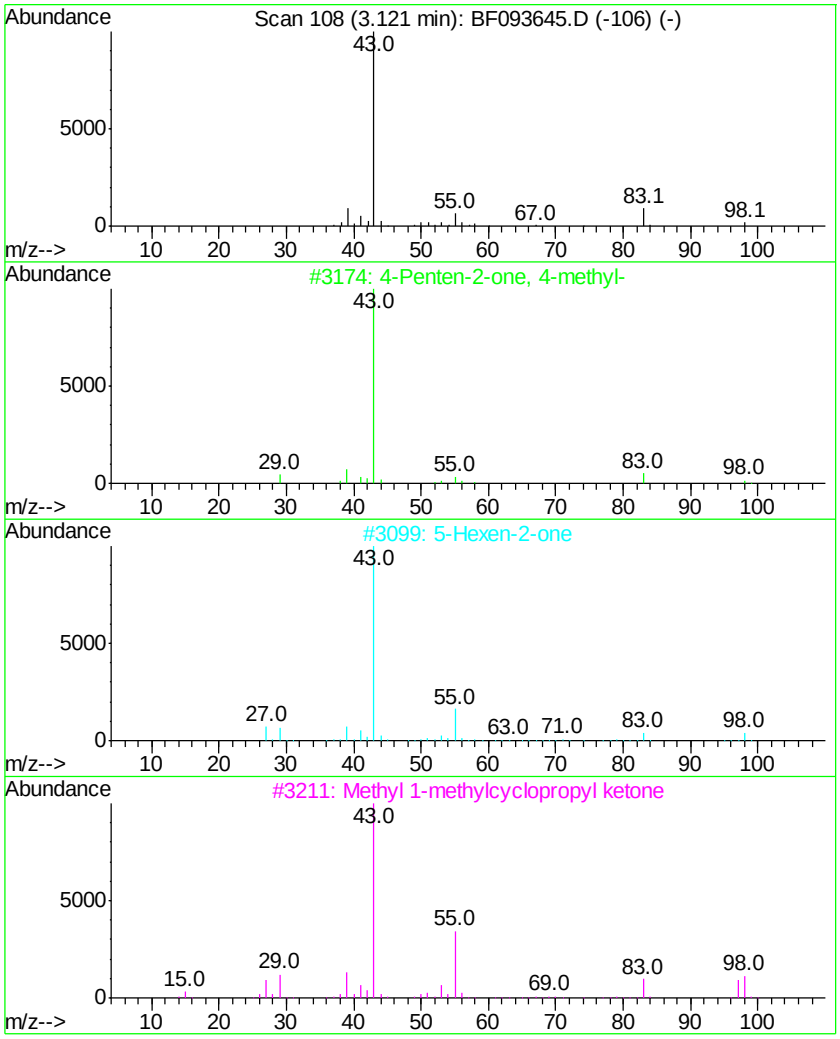
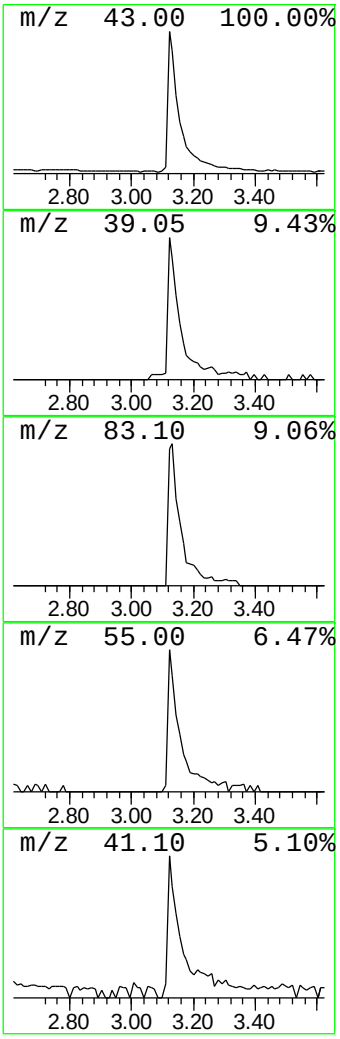
Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.12	8.97 ng	455665	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	80
2	5-Hexen-2-one	98	C6H10O	000109-49-9	46
3	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	37
4	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	37
5	Pent-3-enylamine	85	C5H11N	087156-70-5	9





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ClientSampleId : D-121

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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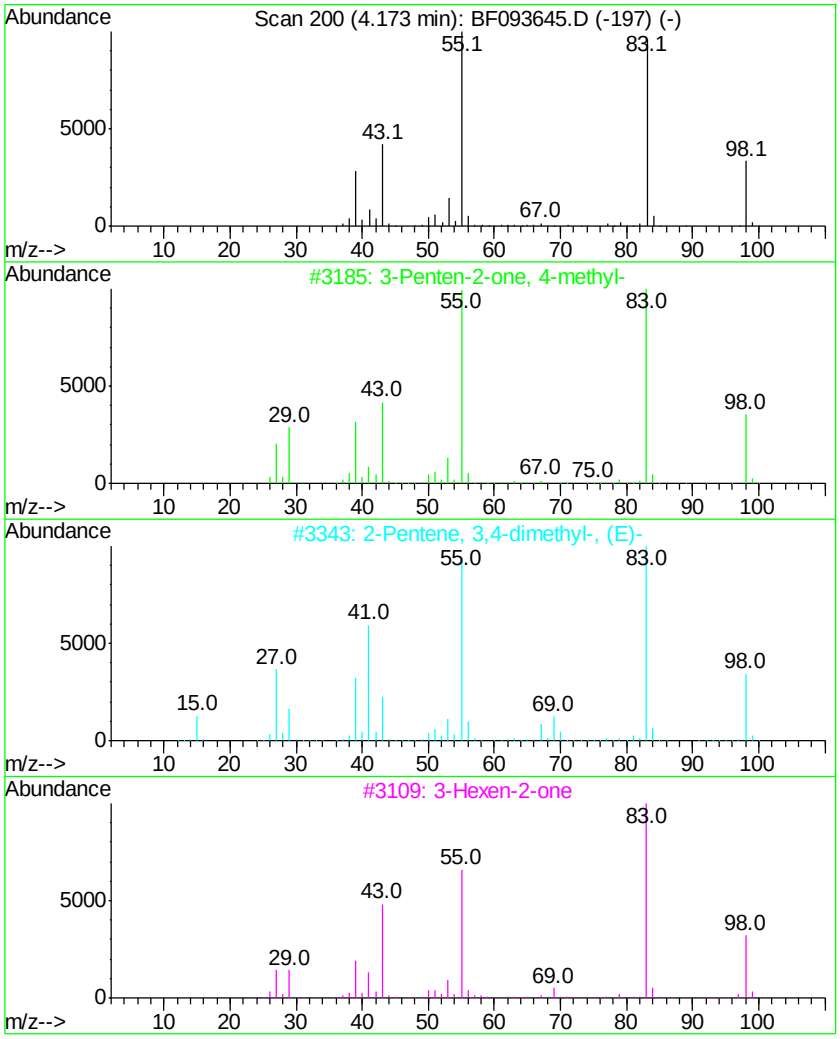
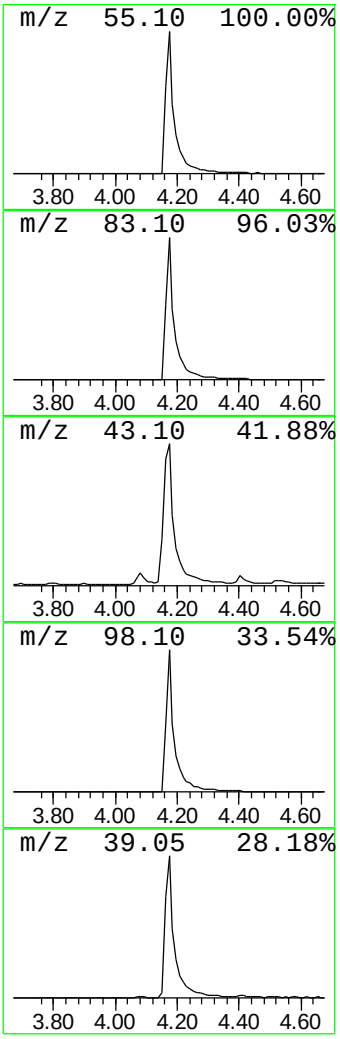
Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.17	47.46 ng	2411800	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3	3-Hexen-2-one	98	C6H10O	000763-93-9	87
4	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





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Instrument : BNA_F
ClientSampleId : D-121

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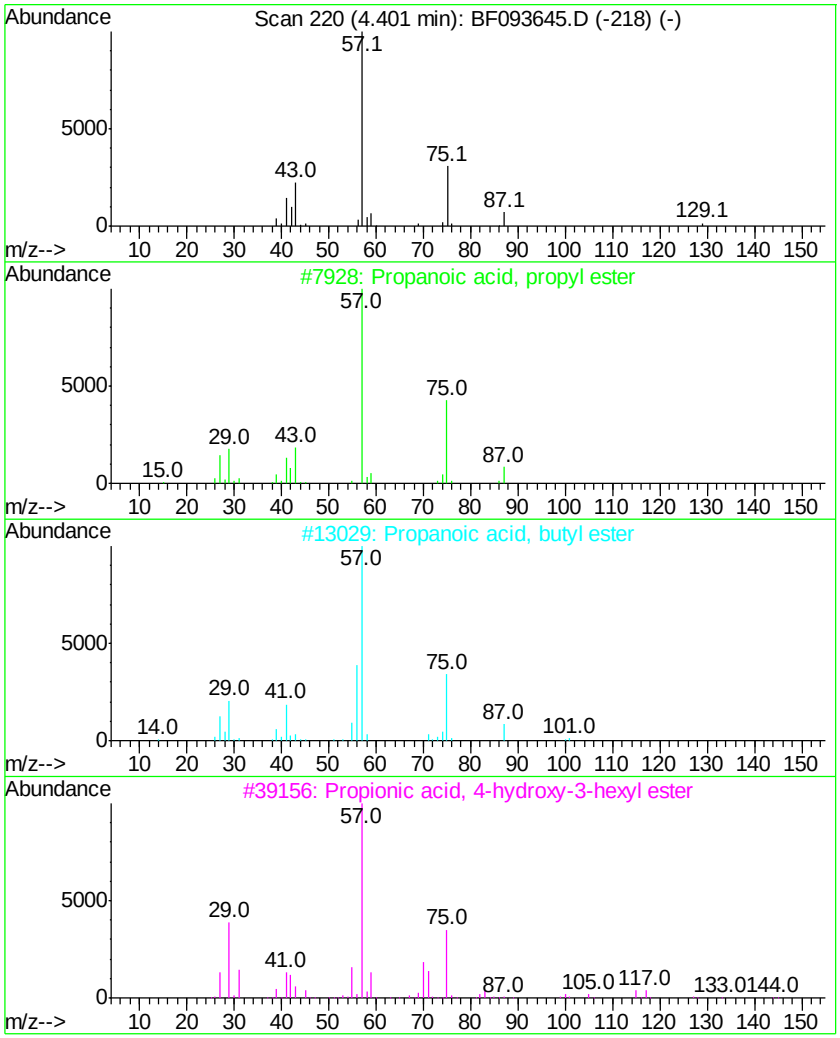
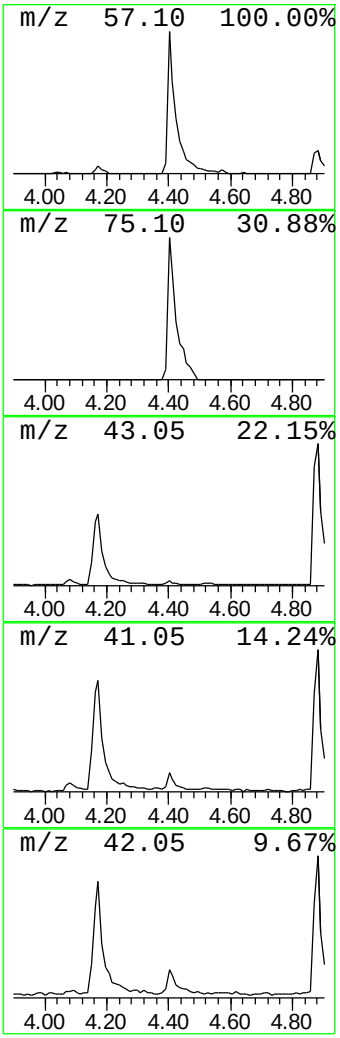
Peak Number 4 Propanoic acid, propyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	2.05 ng	104406	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
2	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	9
3	Propionic acid, 4-hydroxy-3-hexy...	174	C9H18O3	1000151-16-9	9
4	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
5	Azetidine	57	C3H7N	000503-29-7	7





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Sample : I2201-21
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Instrument : BNA_F
ClientSampleId : D-121

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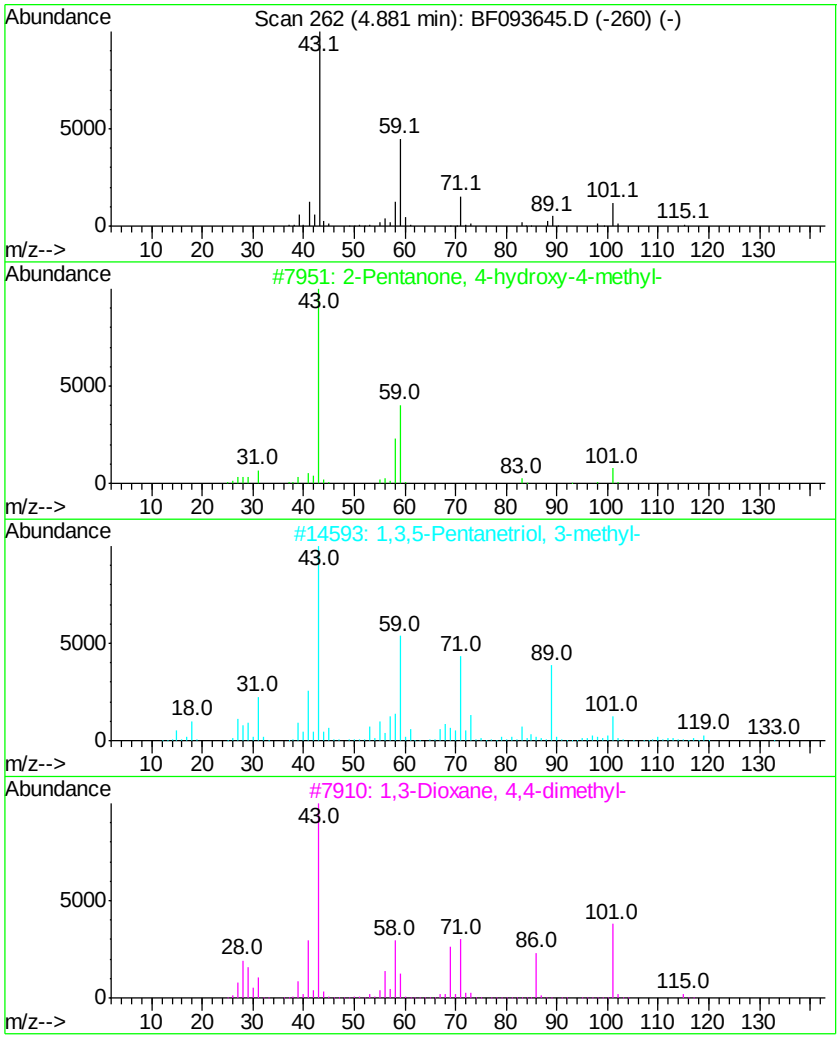
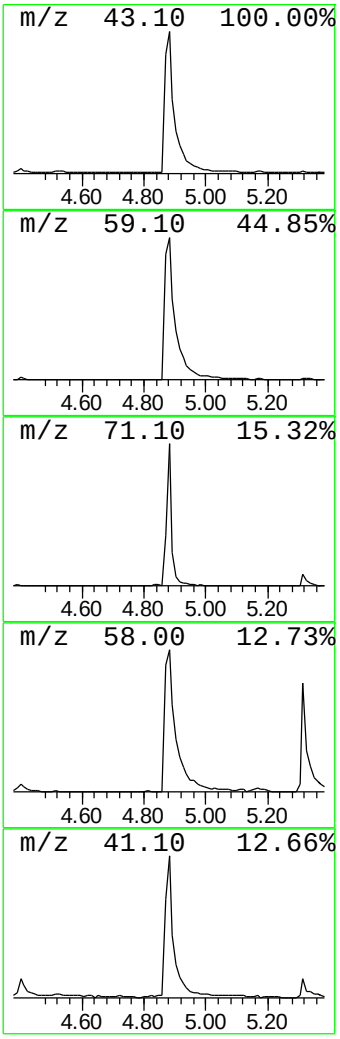
Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	26.97 ng	1370290	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	1,3,5-Pentanetriol, 3-methyl-	134	C6H14O3	007564-64-9	38
3	1,3-Dioxane, 4,4-dimethyl-	116	C6H12O2	000766-15-4	12
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





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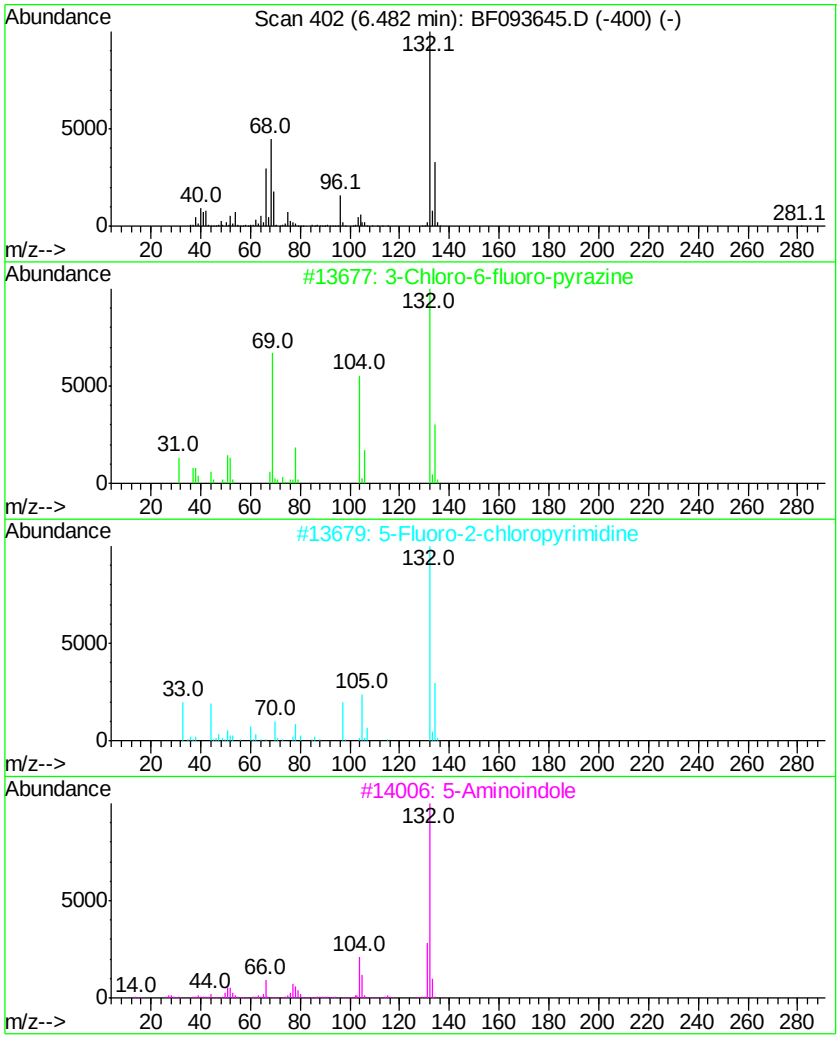
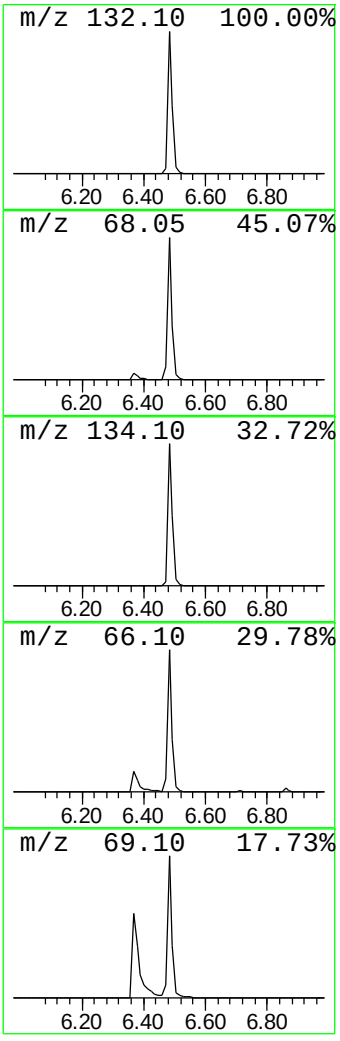
Peak Number 6 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	94.65 ng	4809860	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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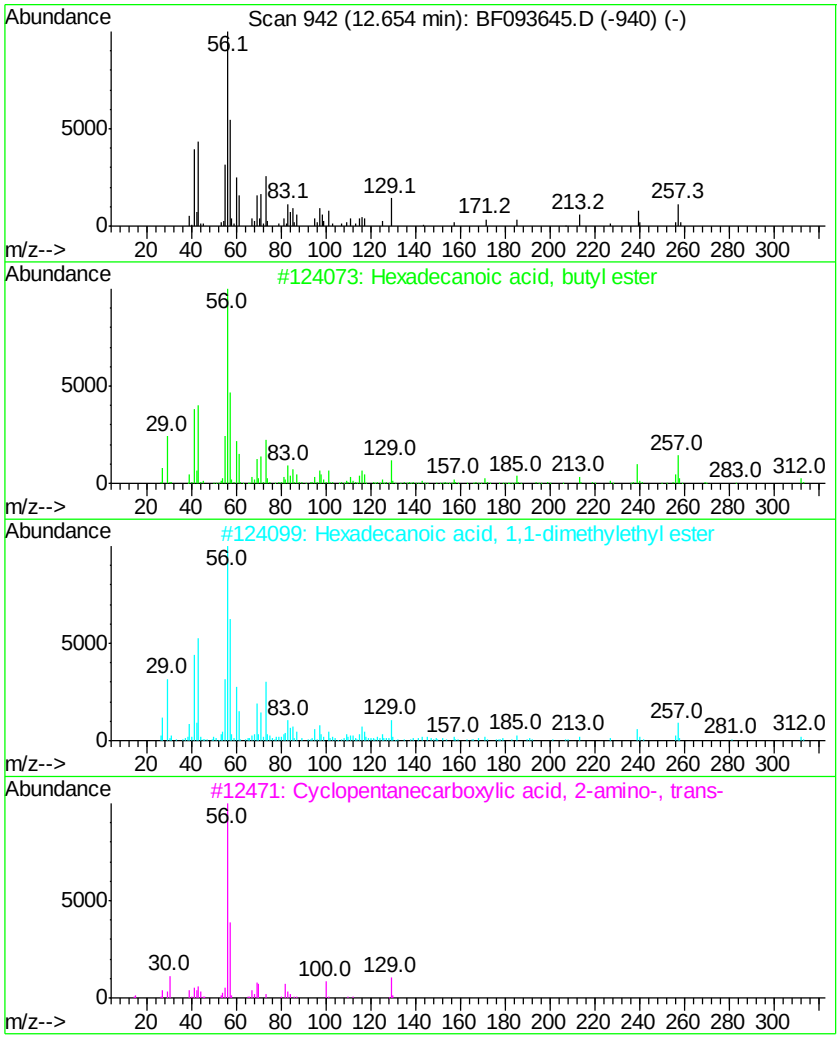
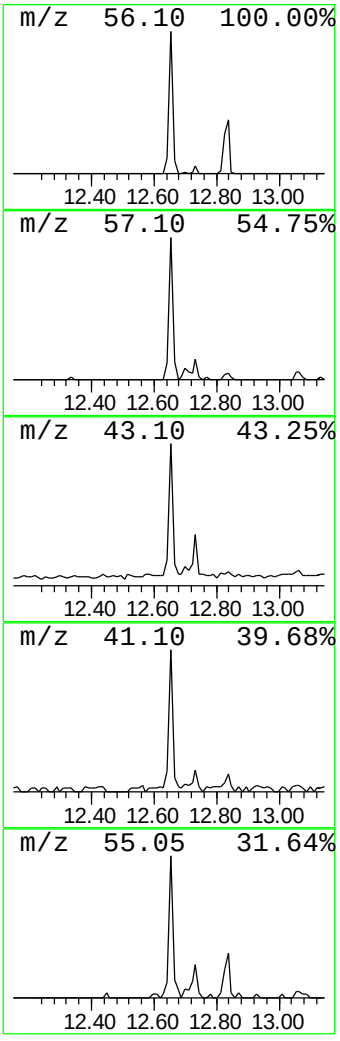
Peak Number 8 Hexadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	2.49 ng	143366	Chrysene-d12	13.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	62
3	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	38
4	1-Pentadecene, 2-methyl-	224	C16H32	029833-69-0	37
5	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	37





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Propyl acetate	2.44	4.4	ng	223826	1	6.71	1016340	20.0
4-Penten-2-one, 4...	3.12	9.0	ng	455665	1	6.71	1016340	20.0
3-Penten-2-one, 4...	4.17	47.5	ng	2411800	1	6.71	1016340	20.0
Propanoic acid, p...	4.40	2.0	ng	104406	1	6.71	1016340	20.0
2-Pentanone, 4-hy...	4.88	27.0	ng	1370290	1	6.71	1016340	20.0
unknown6.48	6.48	94.7	ng	4809860	1	6.71	1016340	20.0
Hexadecanoic acid...	12.65	2.5	ng	143366	5	13.90	1153720	20.0