LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072121\
Data File : BF124679.D
Acq On : 22 Jul 2021 2:15
Operator : JU/CG
Sample : M3109-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PX-02D

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124682.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	13	17	21	rBB	13441	16866	6.19%	1.097%
2	5.122	514	516	521	rBB	4165	4818	1.77%	0.313%
3	5.504	576	581	584	rBB	173347	186610	68.52%	12.134%
4	6.510	747	752	755	rBB	168040	192327	70.62%	12.506%
5	6.887	813	816	819	rBB	44610	32913	12.09%	2.140%
6	7.451	907	912	915	rBB	136125	129917	47.70%	8.448%
7	8.069	1014	1017	1019	rBB	11294	8516	3.13%	0.554%
8	8.169	1030	1034	1037	rBB	58637	45570	16.73%	2.963%
9	9.251	1213	1218	1221	rBB	306951	265623	97.53%	17.272%
10	9.928	1330	1333	1336	rBB	73547	55207	20.27%	3.590%
11	10.716	1463	1467	1470	rBB	184441	167346	61.45%	10.882%
12	11.416	1582	1586	1589	rBB	71078	57226	21.01%	3.721%
13	11.933	1672	1674	1676	rBB	18451	11606	4.26%	0.755%
14	12.722	1805	1808	1810	rBB	7390	5421	1.99%	0.352%
15	13.004	1851	1856	1859	rBV	294217	272345	100.00%	17.709%
16	13.898	2005	2008	2012	rBB	8565	9306	3.42%	0.605%
17	14.051	2031	2034	2037	rBB	47619	37044	13.60%	2.409%
18	14.216	2059	2062	2064	rBB	4218	3545	1.30%	0.231%
19	14.516	2111	2113	2116	rBB	3826	3142	1.15%	0.204%
20	15.533	2281	2286	2289	rBB	29222	32528	11.94%	2.115%

Sum of corrected areas: 1537876

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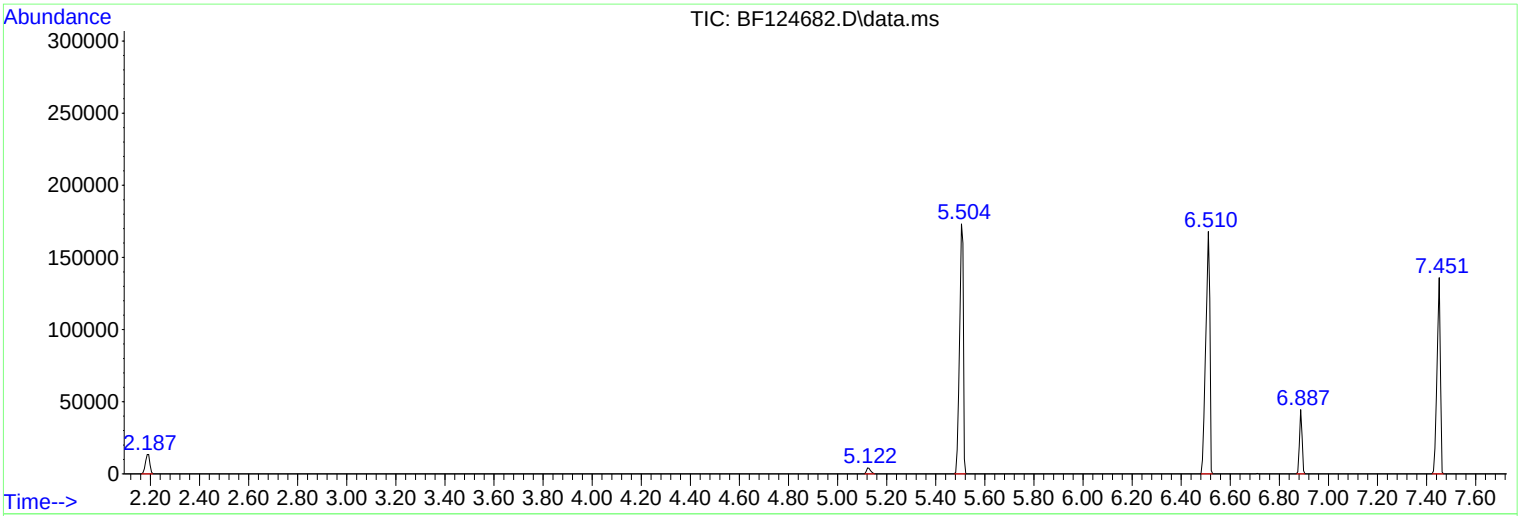
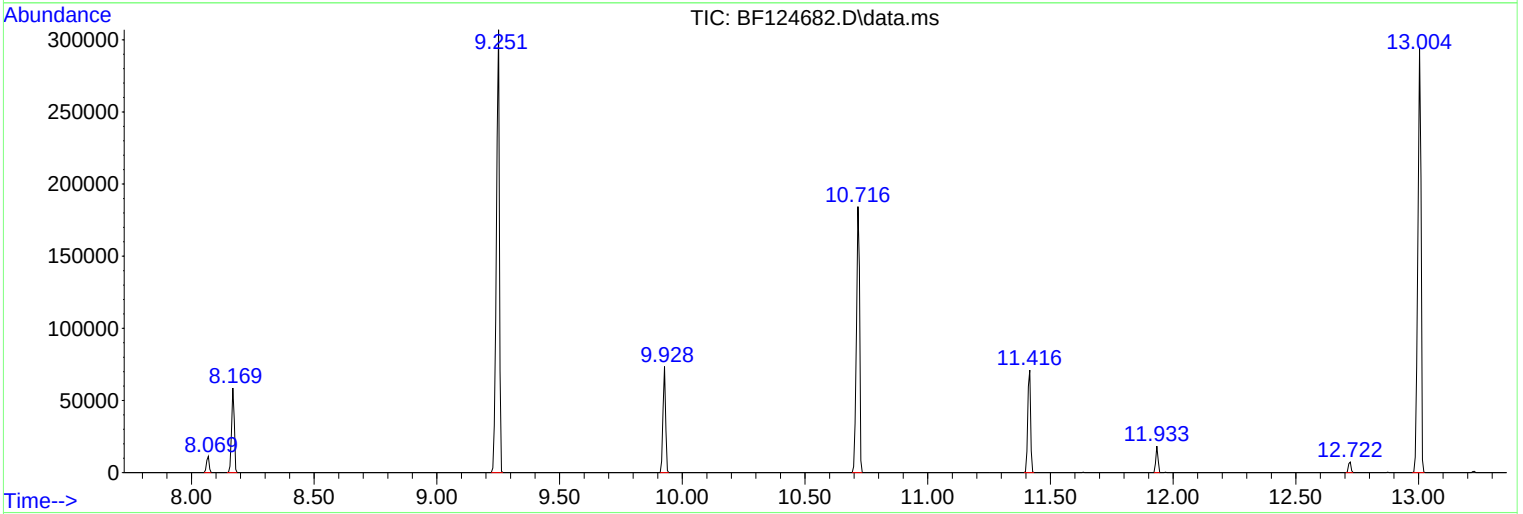
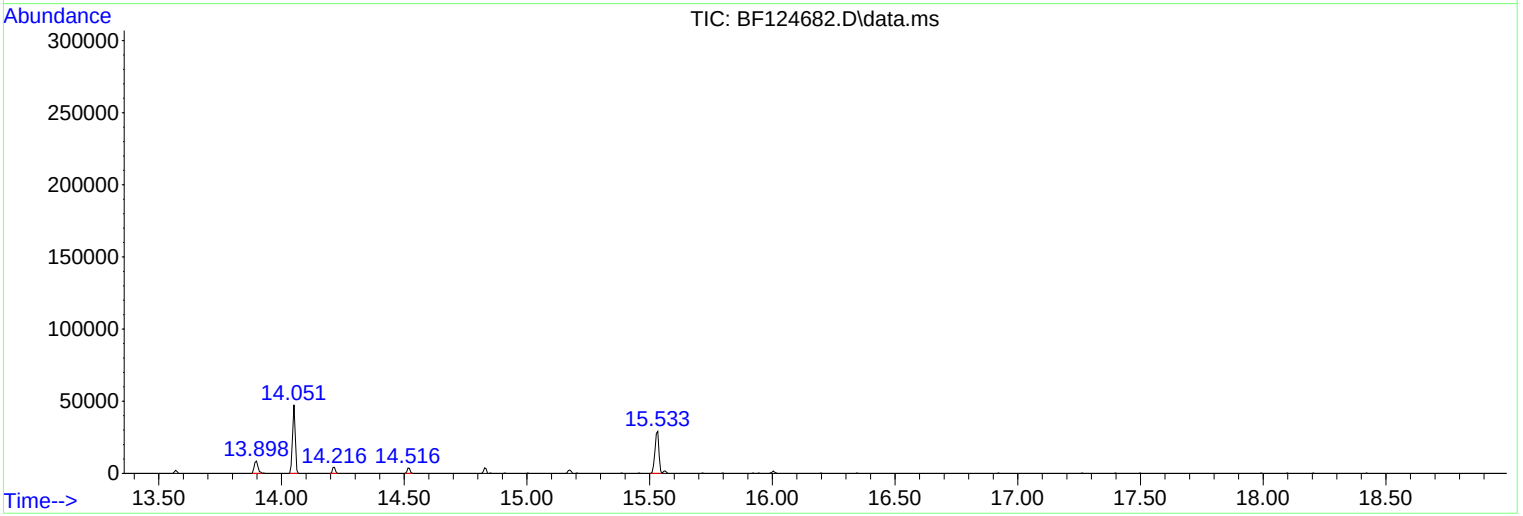
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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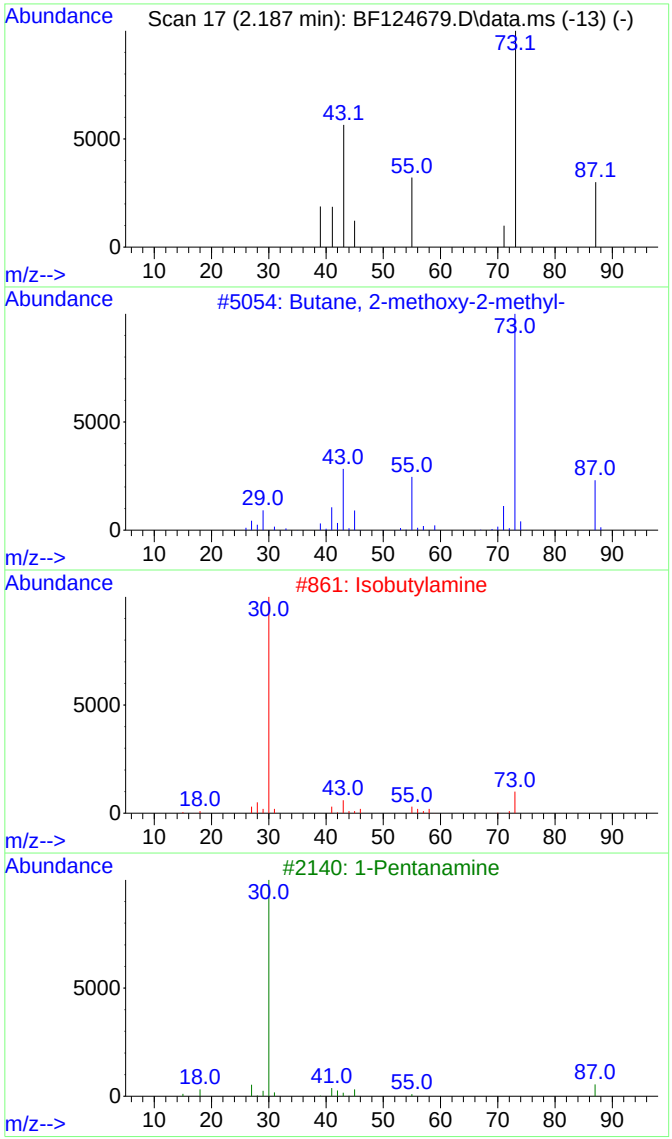
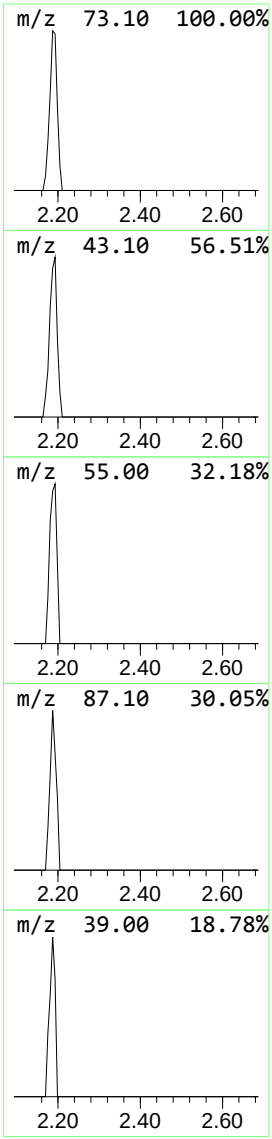
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.187	10.25 ng	16866	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	Isobutylamine	73	C4H11N	000078-81-9	5
3	1-Pentanamine	87	C5H13N	000110-58-7	4
4	3,4-Hexanediol, 2,5-dimethyl-	146	C8H18O2	022607-11-0	4
5	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	4





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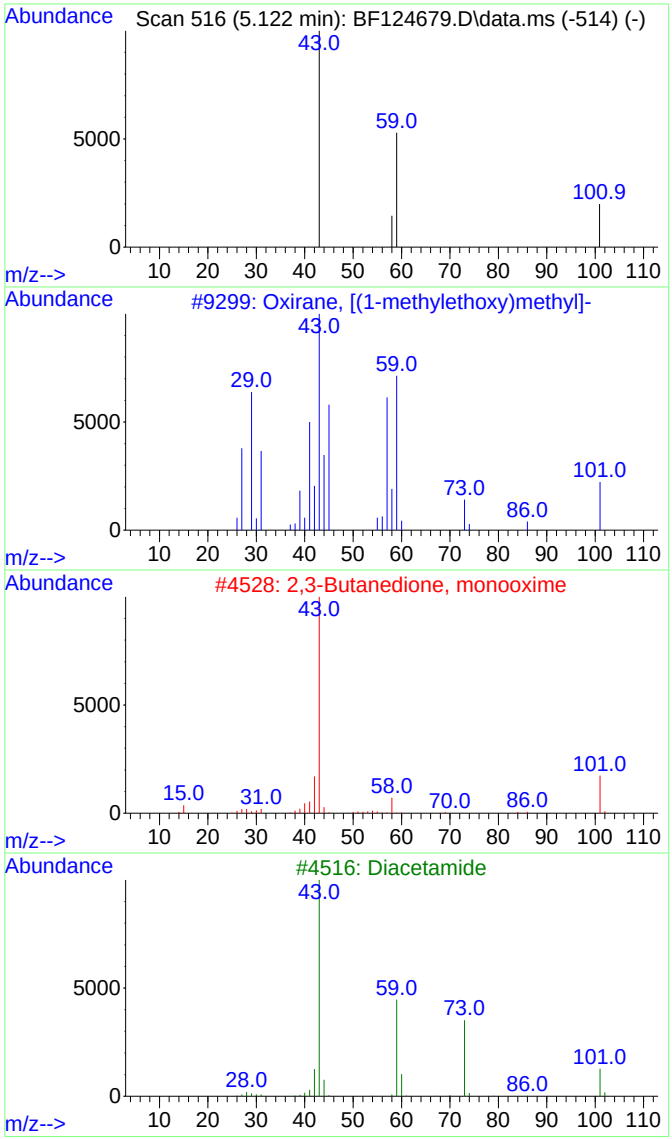
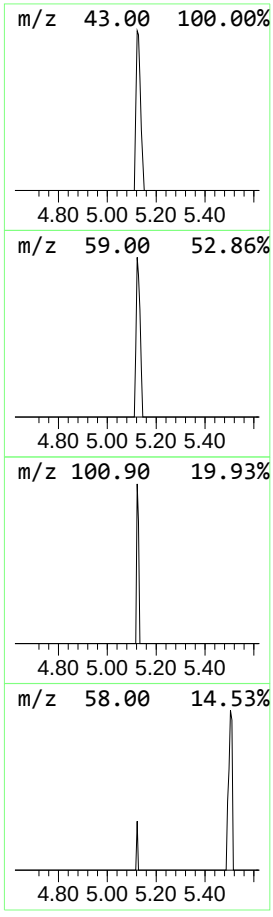
Peak Number 2 unknown5.122 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.122	2.93 ng	4818	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	9
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	5
3	Diacetamide	101	C4H7NO2	000625-77-4	4
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	4
5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	4





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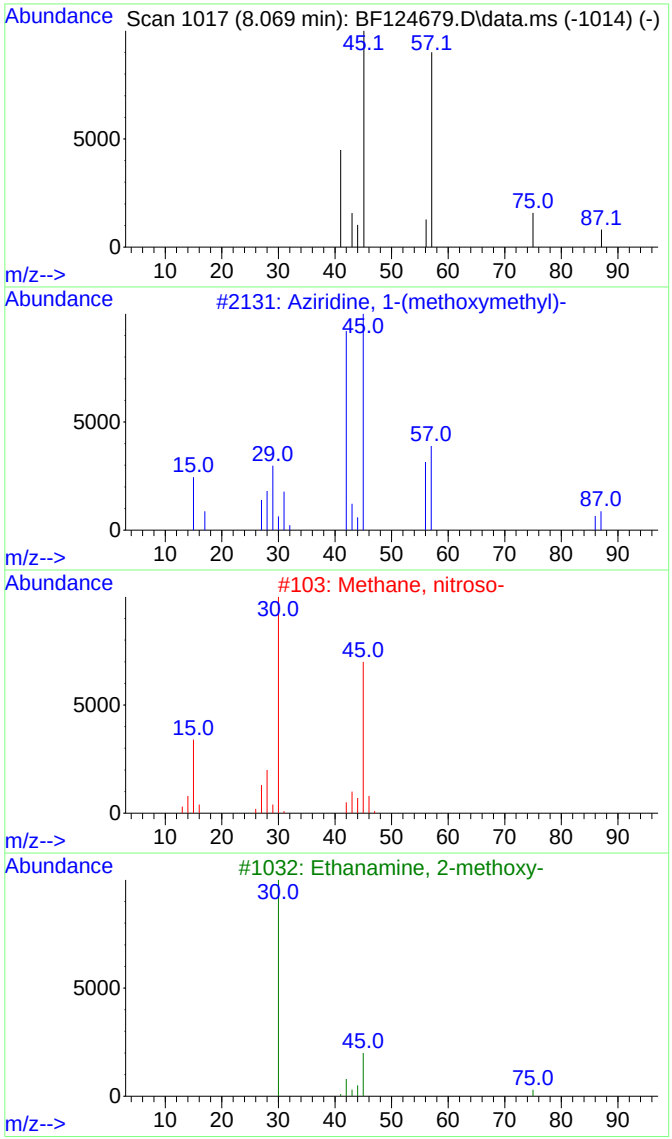
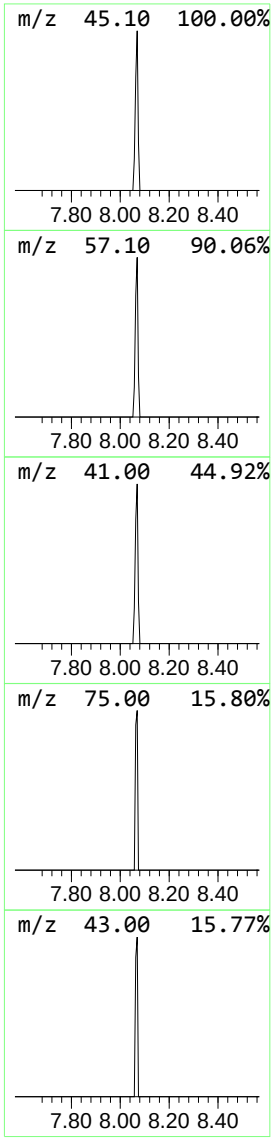
Peak Number 3 unknown8.069 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.069	3.74 ng	8516	Naphthalene-d8	8.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aziridine, 1-(methoxymethyl)-	87	C4H9NO	001497-83-2	7
2	Methane, nitroso-	45	CH3NO	000865-40-7	4
3	Ethanamine, 2-methoxy-	75	C3H9NO	000109-85-3	4
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	4
5	Propanedioic acid, oxo-, bis(2-m...	230	C11H18O5	092778-43-3	4





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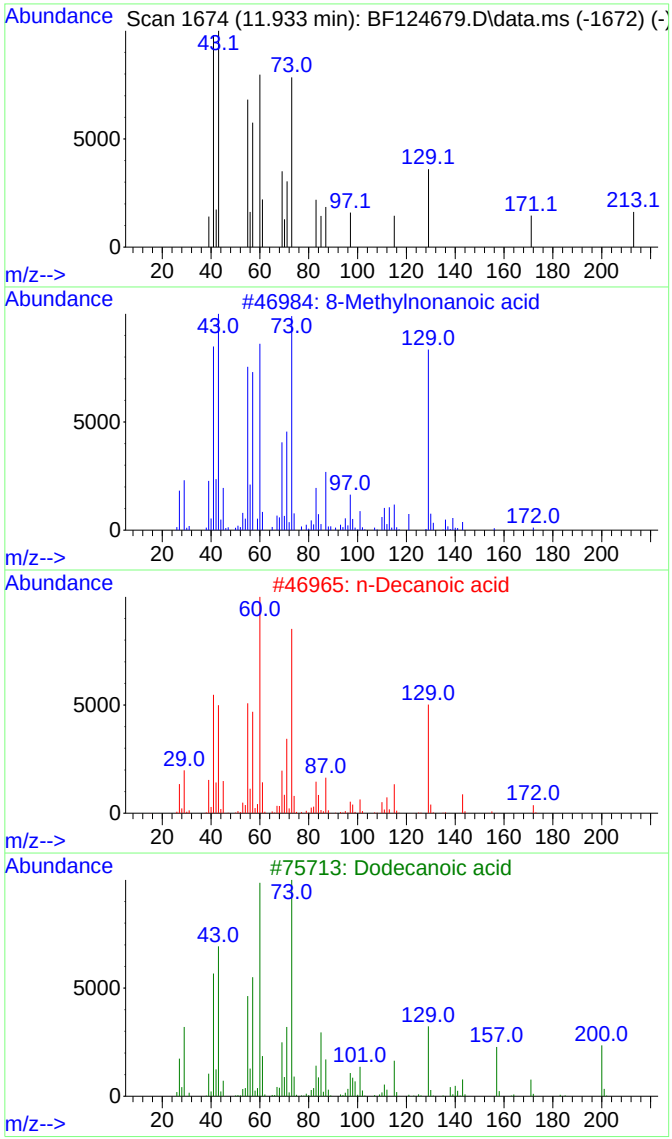
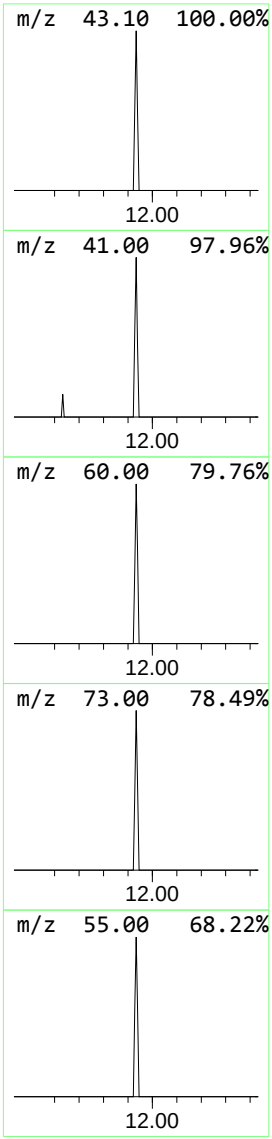
Peak Number 4 8-Methylnonanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	4.06 ng	11606	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	58
2	n-Decanoic acid	172	C10H20O2	000334-48-5	53
3	Dodecanoic acid	200	C12H24O2	000143-07-7	53
4	.beta.-D-Glucopyranoside, methyl...	292	C14H28O6	1010157-04-9	42
5	Undecanedioic acid, monomethyl e...	230	C12H22O4	003927-60-4	14





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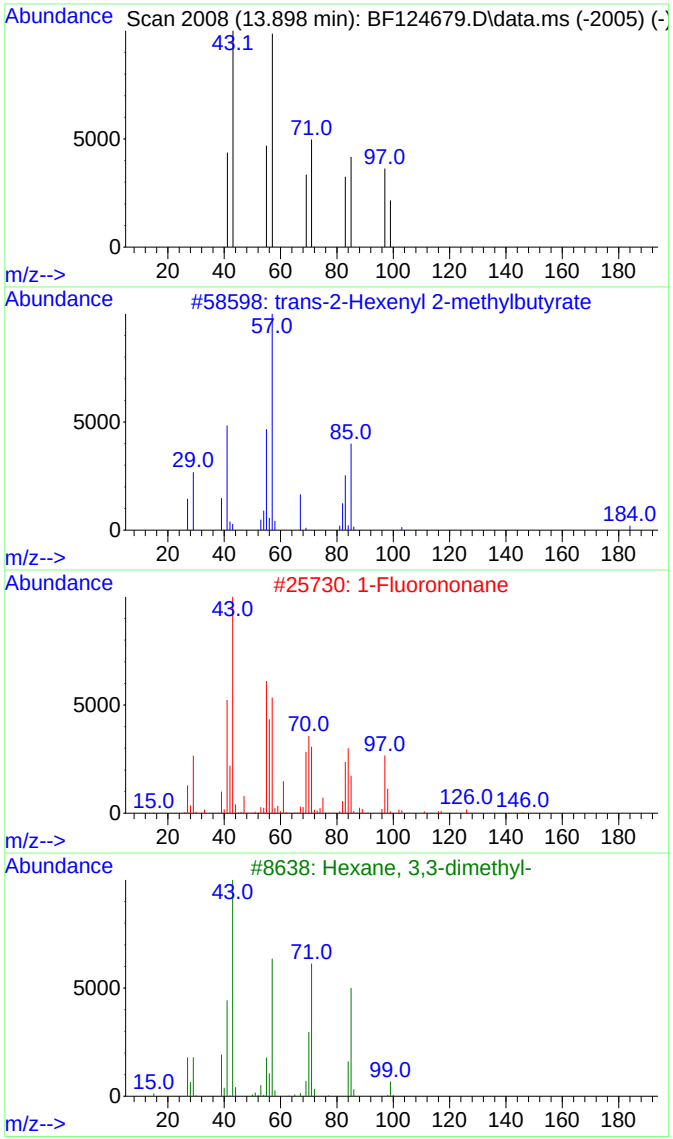
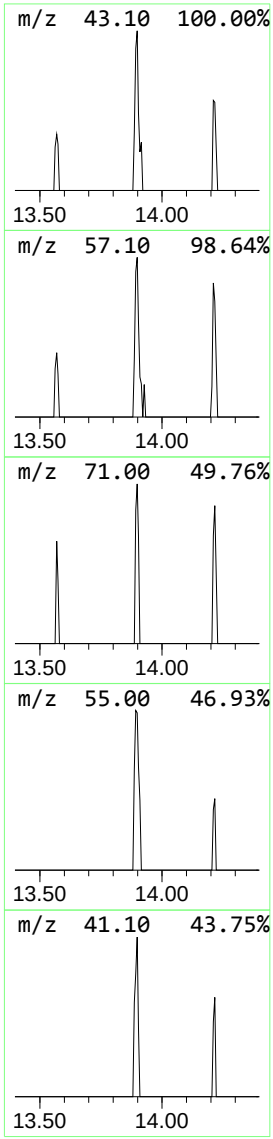
Peak Number 5 unknown13.898 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	5.02 ng	9306	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-2-Hexenyl 2-methylbutyrate	184	C11H20O2	1000433-23-8	23
2	1-Fluorononane	146	C9H19F	000463-18-3	9
3	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	9
4	Hexane, 1-(hexyloxy)-3-methyl-	200	C13H28O	074421-18-4	9
5	1-Pentanol, 2,3-dimethyl-	116	C7H16O	010143-23-4	9





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
Butane, 2-metho...	2.187	10.3	ng	16866	1	6.887	32913	20.0
unknown5.122	5.122	2.9	ng	4818	1	6.887	32913	20.0
unknown8.069	8.069	3.7	ng	8516	2	8.169	45570	20.0
8-Methylnonanoi...	11.933	4.1	ng	11606	4	11.416	57226	20.0
unknown13.898	13.898	5.0	ng	9306	5	14.051	37044	20.0