LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090624\
Data File : BF139275.D
Acq On : 06 Sep 2024 14:02
Operator : RC/JU
Sample : P3852-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI356

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-BF090424.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139275.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	6	13	rVB	1419676	1964945	100.00%	14.308%
2	5.087	501	509	517	rVB	85324	133353	6.79%	0.971%
3	5.498	571	579	584	rBV	1214281	1655102	84.23%	12.052%
4	6.510	746	751	764	rVB	1206698	1641735	83.55%	11.954%
5	6.886	801	815	823	rBV2	607467	910693	46.35%	6.631%
6	6.986	824	832	836	rBV3	60903	159211	8.10%	1.159%
7	7.445	902	910	915	rBV	805732	1015930	51.70%	7.398%
8	8.169	1027	1033	1038	rBV	600974	781775	39.79%	5.693%
9	8.498	1085	1089	1095	rVB	93133	133087	6.77%	0.969%
10	8.863	1147	1151	1158	rBV2	208844	342715	17.44%	2.496%
11	9.057	1180	1184	1192	rBV4	131457	278369	14.17%	2.027%
12	9.245	1211	1216	1220	rVB	1230994	1481371	75.39%	10.787%
13	9.327	1226	1230	1235	rBV4	182492	353025	17.97%	2.571%
14	9.592	1271	1275	1279	rBV	691931	883381	44.96%	6.432%
15	9.645	1280	1284	1288	rVV4	284267	471036	23.97%	3.430%
16	9.745	1298	1301	1305	rBV6	211003	285410	14.53%	2.078%
17	9.839	1314	1317	1320	rVB2	293534	322553	16.42%	2.349%
18	9.927	1329	1332	1336	rVB	731223	919524	46.80%	6.696%

Sum of corrected areas: 13733215

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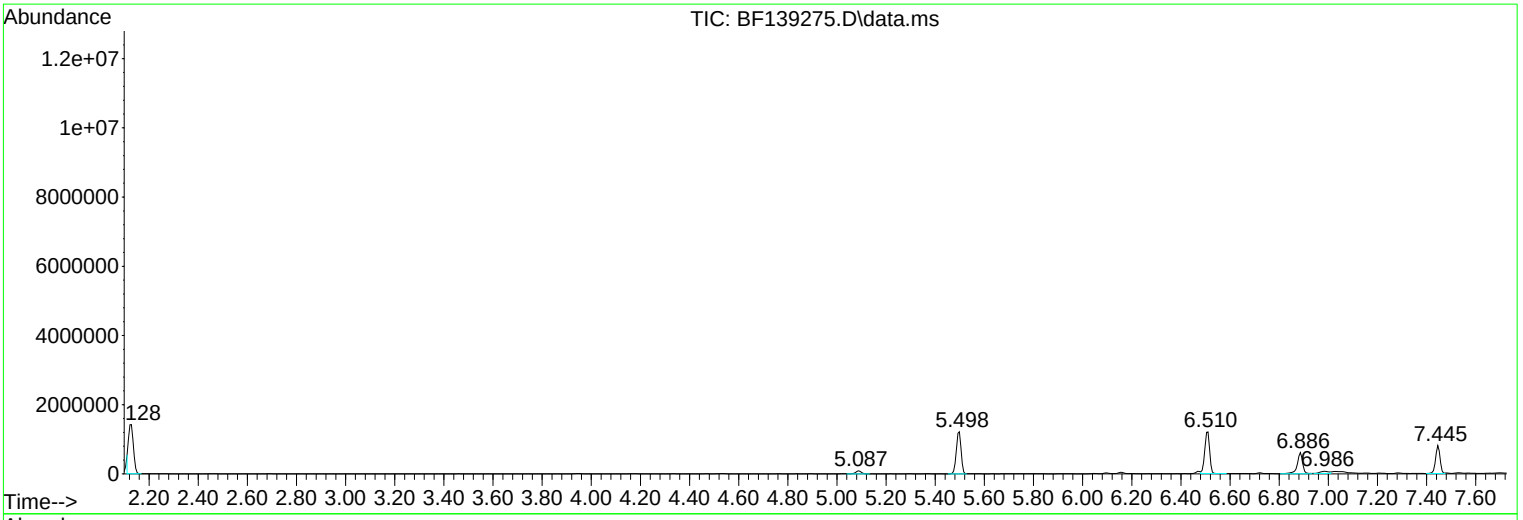
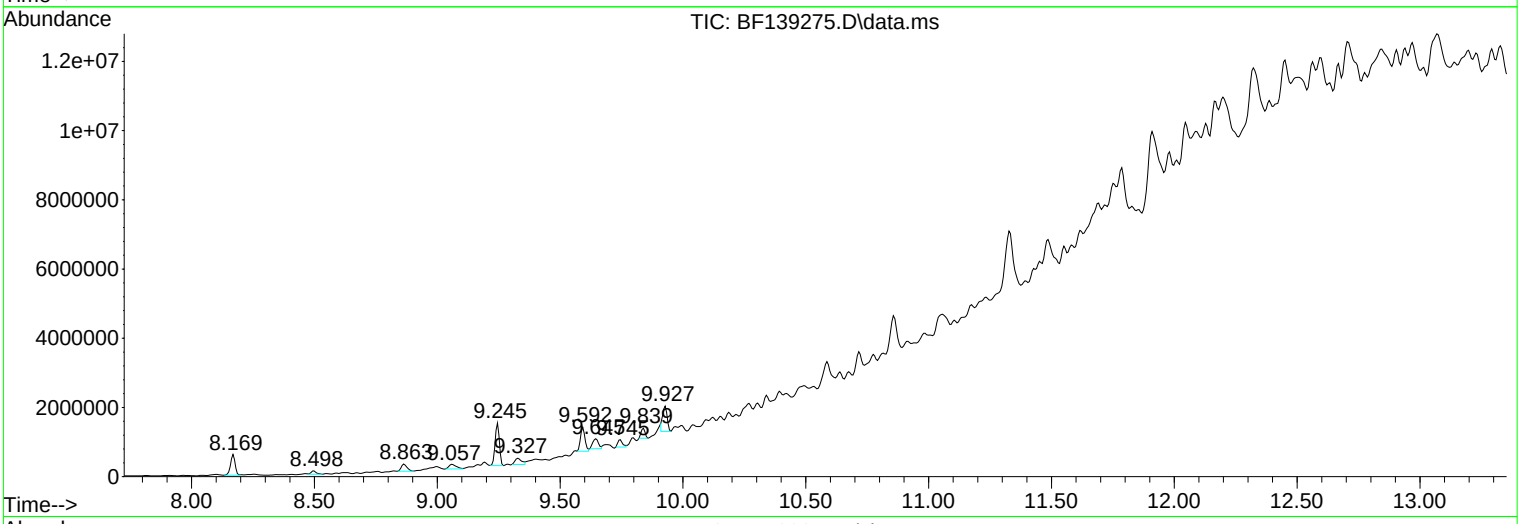
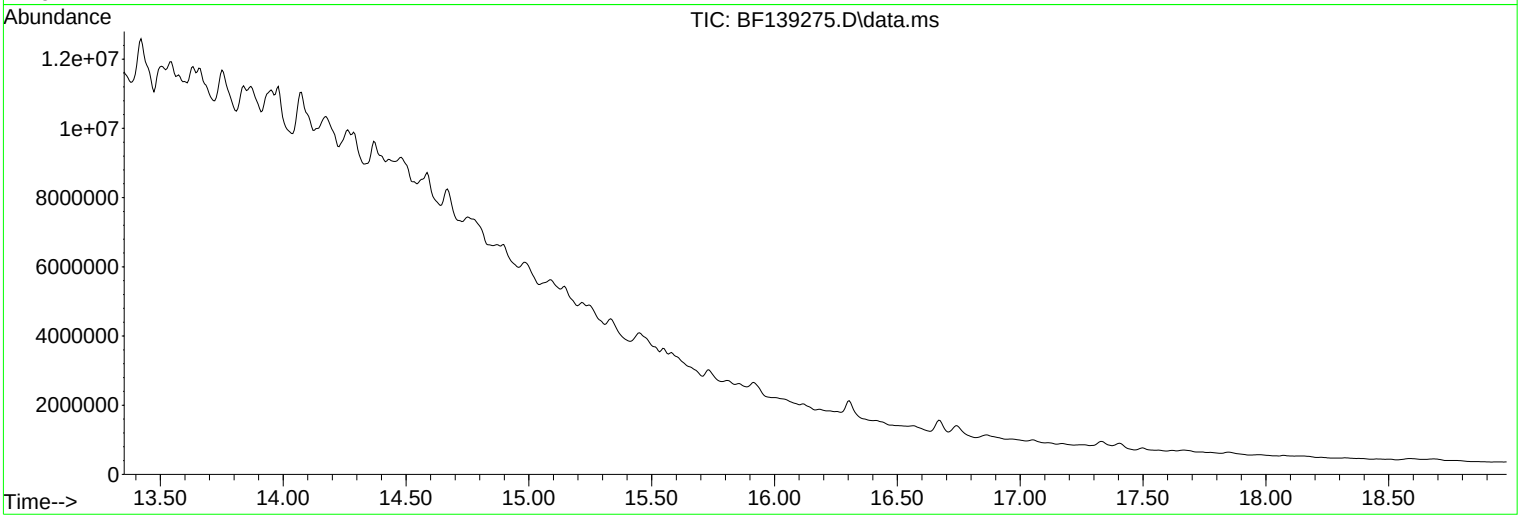
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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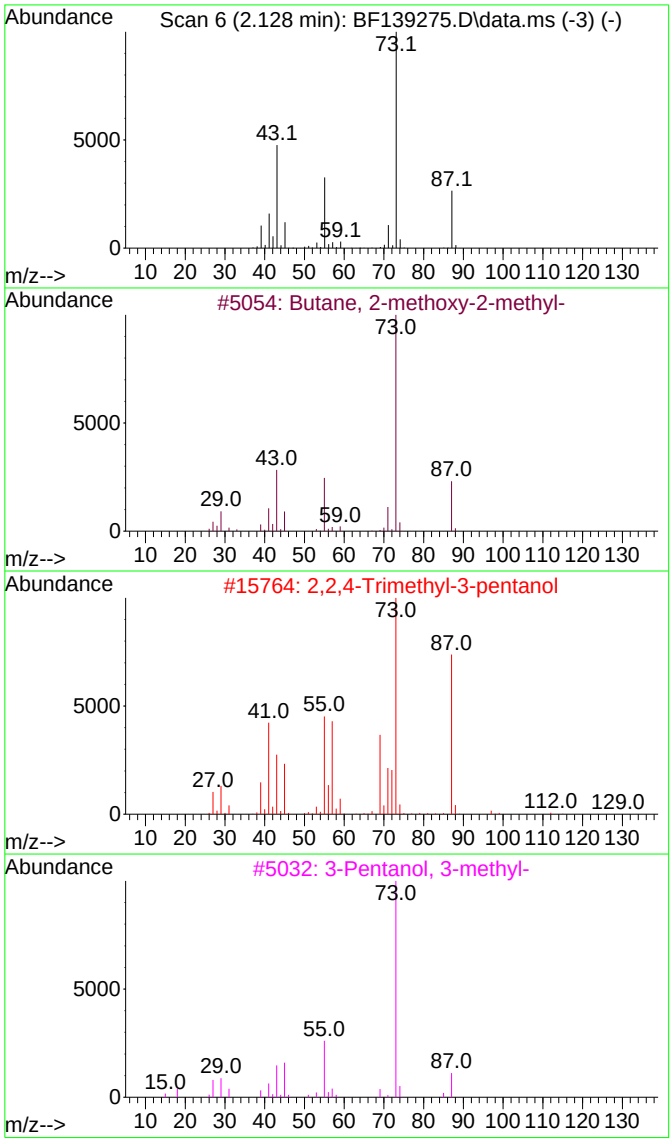
TIC Integration Parameters: LSCINT.P

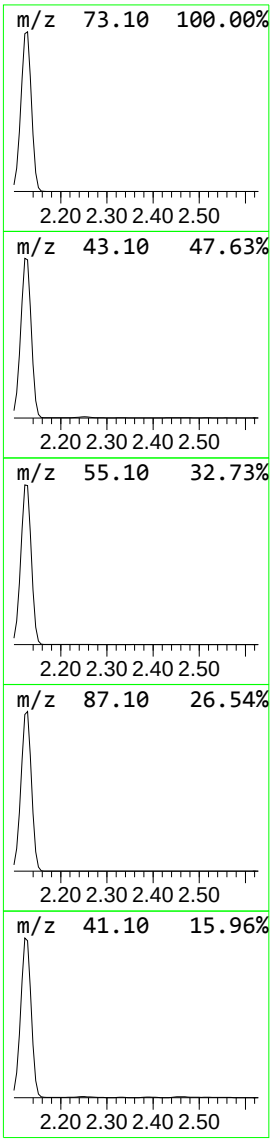
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	43.15 ng	1964950	1,4-Dichlorobenzene-d4	6.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	37
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
5	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	17





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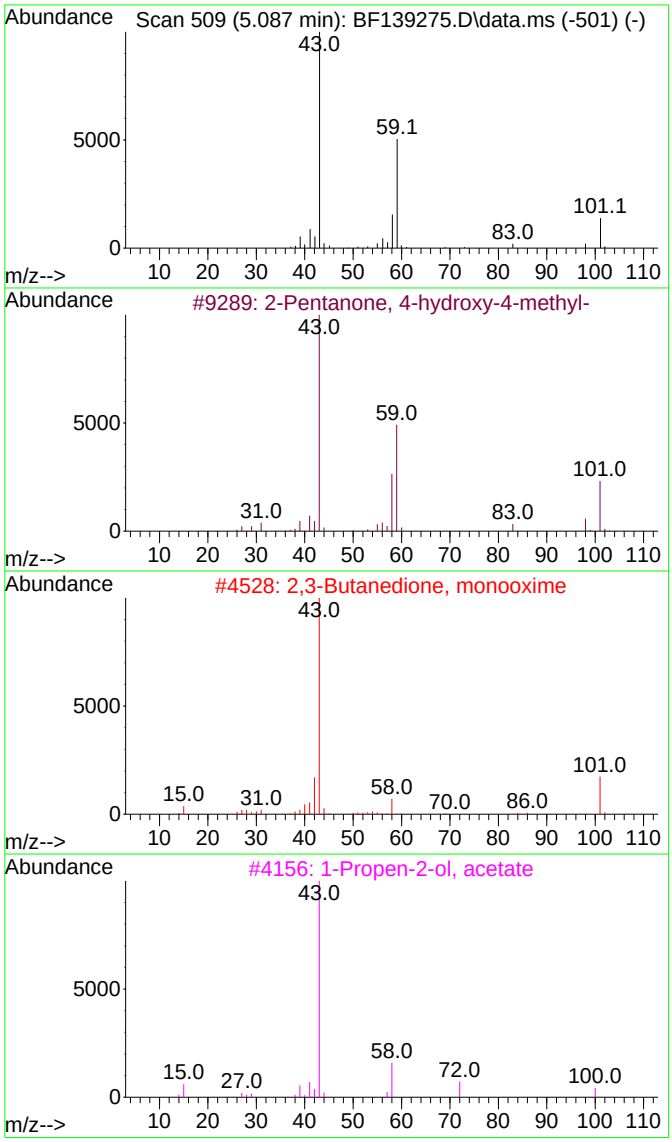
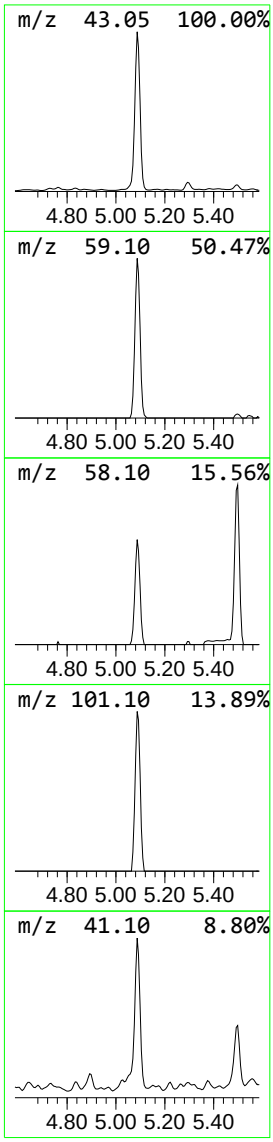
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	2.93 ng	133353	1,4-Dichlorobenzene-d4	6.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	Butane	58	C4H10	000106-97-8	9
5	Diacetamide	101	C4H7NO2	000625-77-4	9





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TIC Integration Parameters: LSCINT.P

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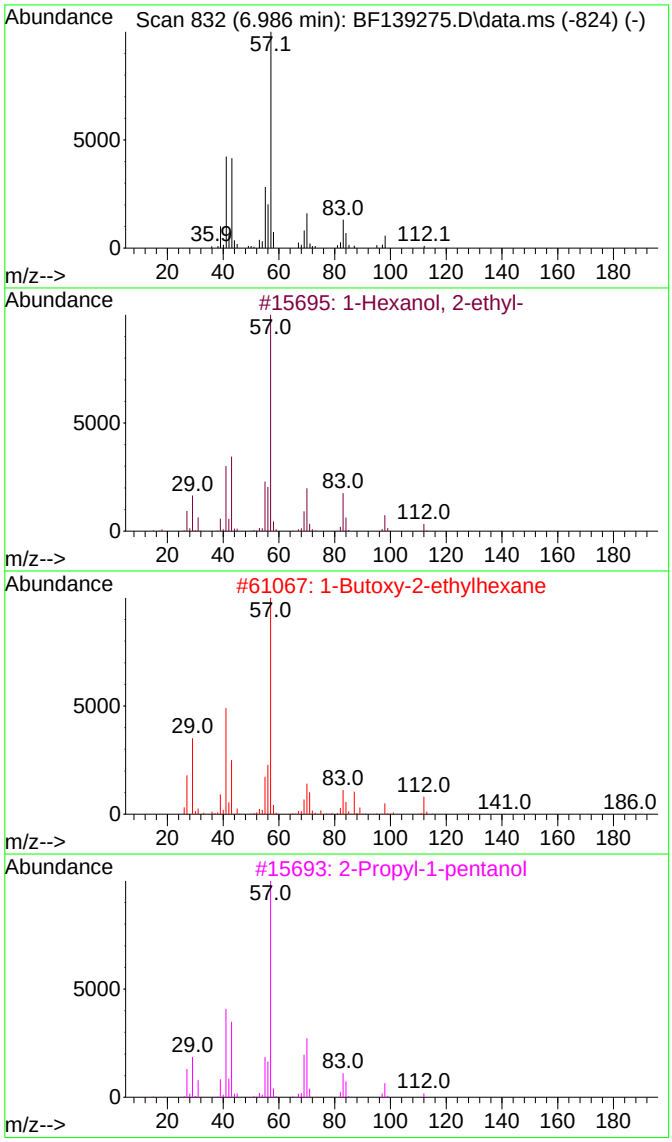
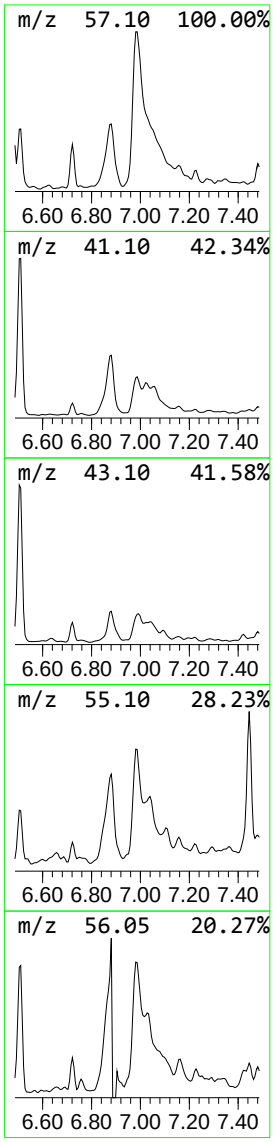
Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.986	3.50 ng	159211	1,4-Dichlorobenzene-d4	6.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2	1-Butoxy-2-ethylhexane	186	C12H26O	062625-25-6	72
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
4	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56
5	2-Propyl-1-Pentanol, trifluoroac...	226	C10H17F3O2	1000365-19-7	53





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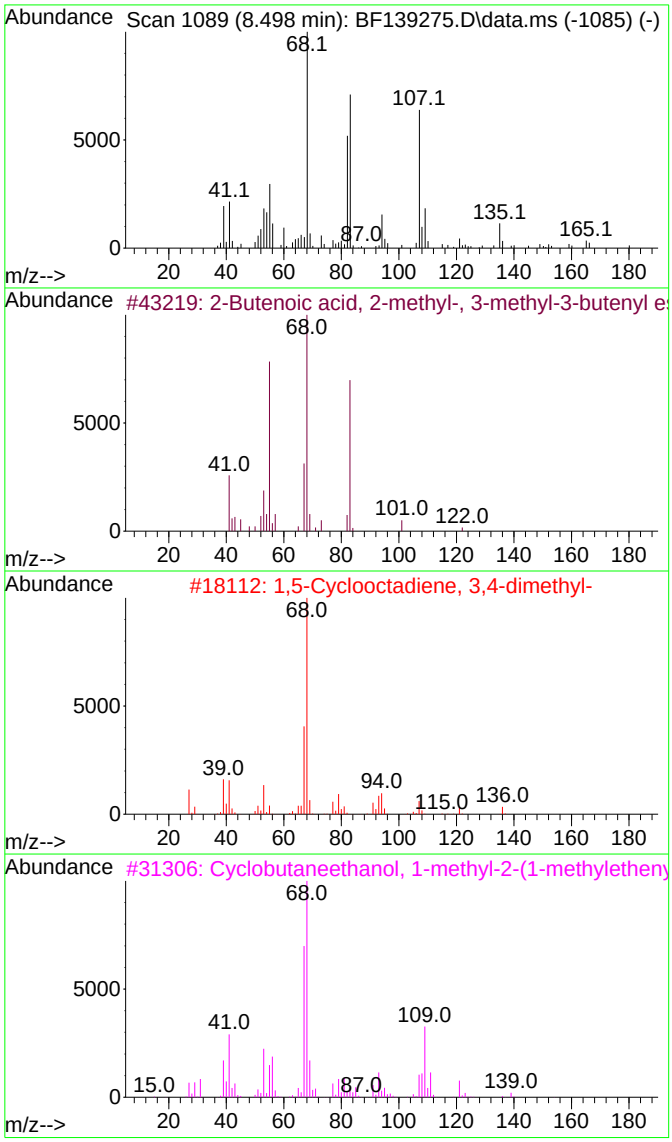
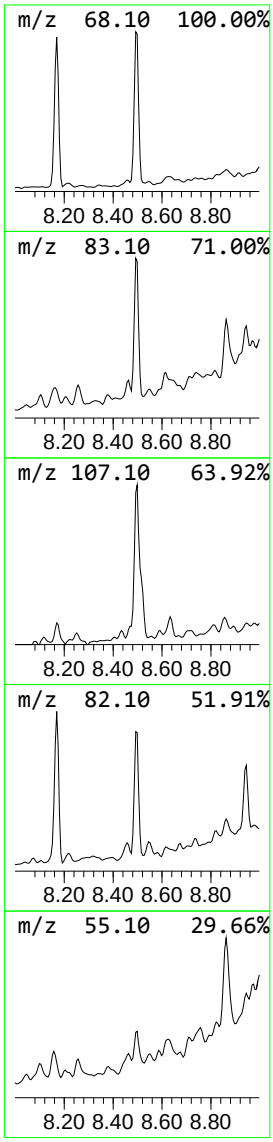
Peak Number 4 unknown8.498 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.498	3.40 ng	133087	Naphthalene-d8	8.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenoic acid, 2-methyl-, 3-me...	168	C10H16O2	083783-87-3	32
2	1,5-Cyclooctadiene, 3,4-dimethyl-	136	C10H16	021284-05-9	22
3	Cyclobutaneethanol, 1-methyl-2-(...	154	C10H18O	030820-22-5	16
4	Cyclohexane, octyl-	196	C14H28	001795-15-9	10
5	7-Oxabicyclo[2.2.1]hept-5-en-2-one	110	C6H6O2	095530-78-2	10





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Sample : P3852-04
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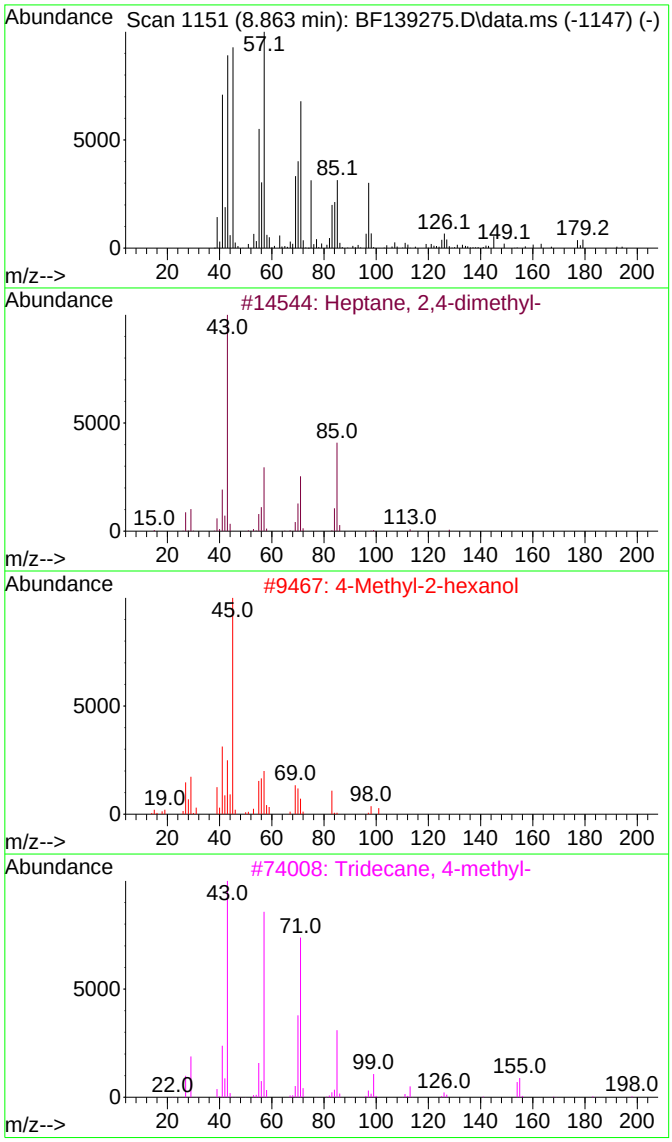
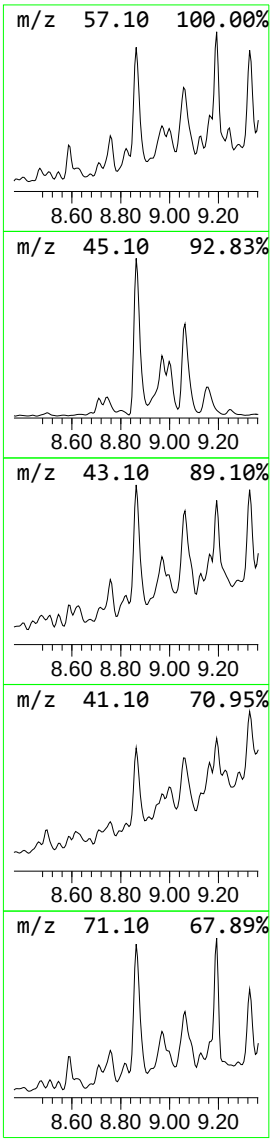
****

Peak Number 5 unknown8.863 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.863	8.77 ng	342715	Naphthalene-d8	8.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	43
2	4-Methyl-2-hexanol	116	C7H16O	002313-61-3	35
3	Tridecane, 4-methyl-	198	C14H30	026730-12-1	27
4	Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	27
5	Octane, 2-methyl-	128	C9H20	003221-61-2	27





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TIC Library : C:\Database\NIST20.L
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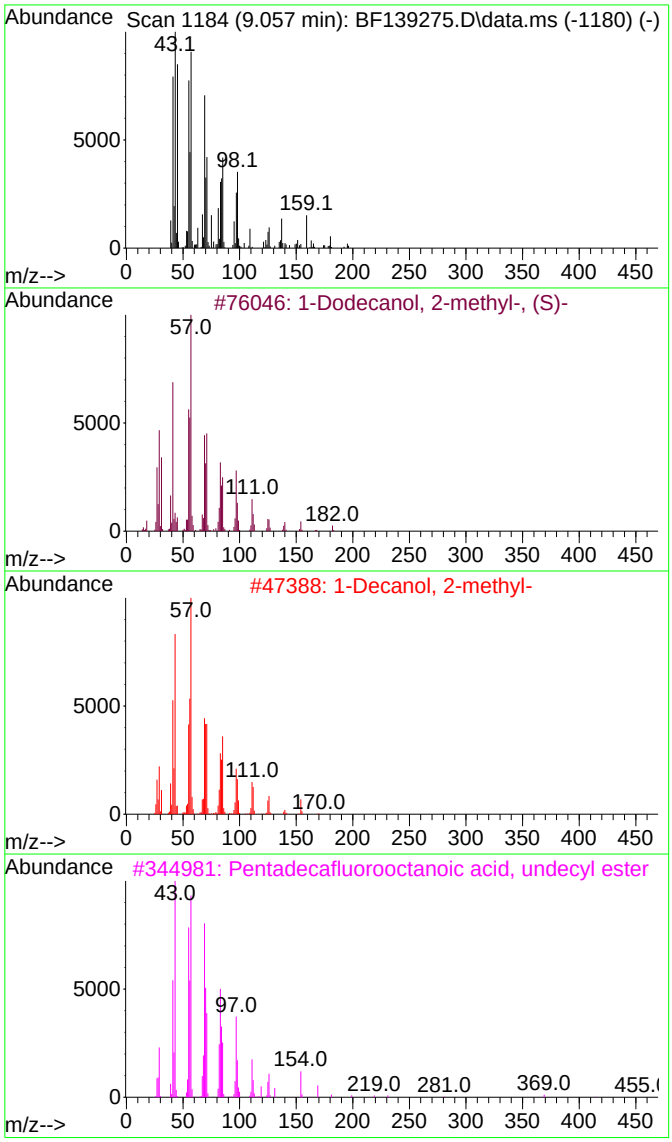
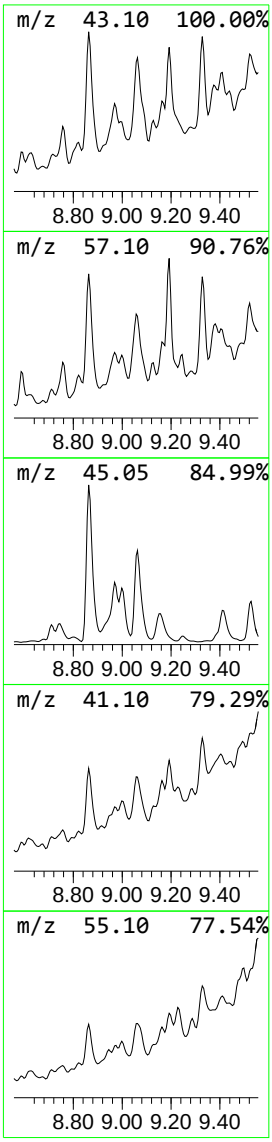
****

Peak Number 6 unknown9.057 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.057	6.05 ng	278369	Acenaphthene-d10	9.927

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-methyl-, (S)-	200	C13H28O	057289-26-6	38
2	1-Decanol, 2-methyl-	172	C11H24O	018675-24-6	35
3	Pentadecafluorooctanoic acid, un...	568	C19H23F15O2	1010406-04-1	35
4	Pentadecane, 6-methyl-	226	C16H34	010105-38-1	27
5	Octane, 4-methyl-	128	C9H20	002216-34-4	27





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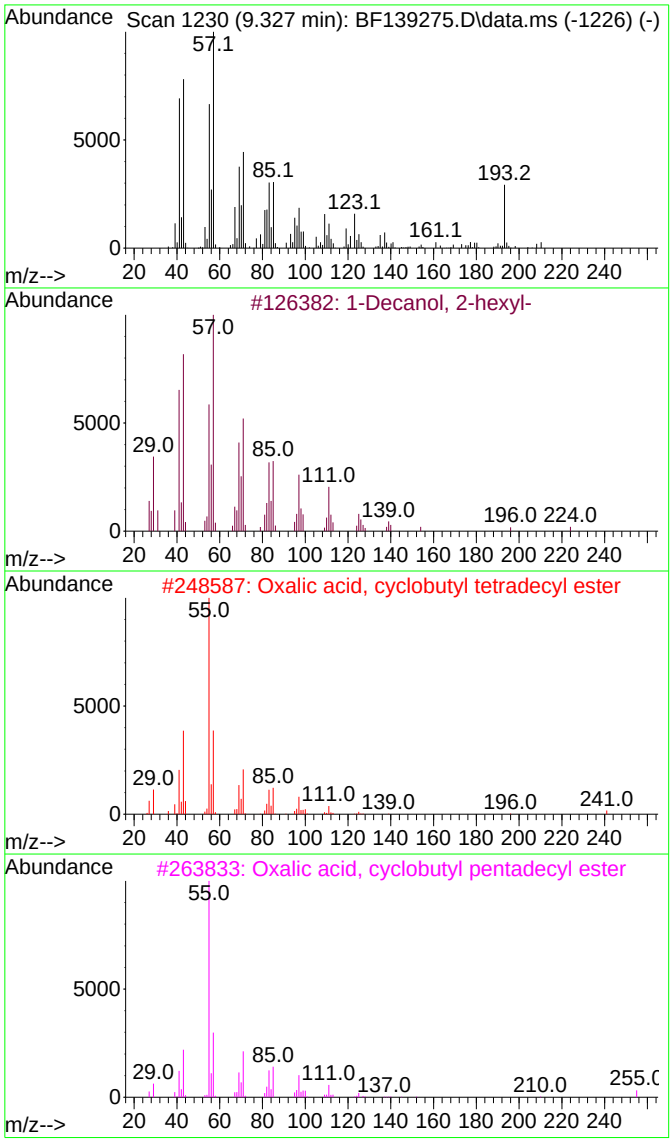
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

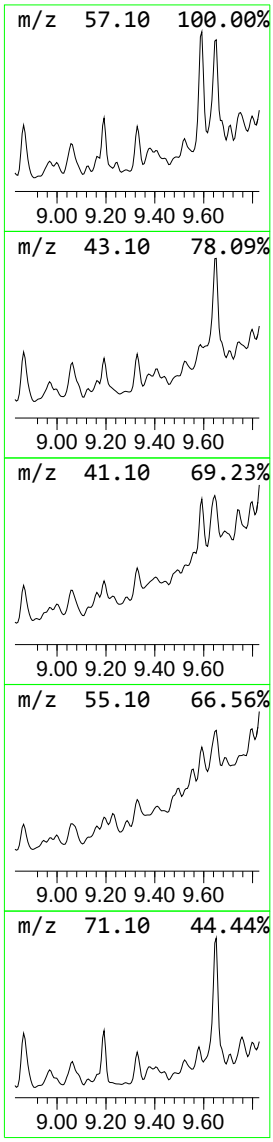
****

Peak Number 7 1-Decanol, 2-hexyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.327	7.68 ng	353025	Acenaphthene-d10	9.927

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	60
2	Oxalic acid, cyclobutyl tetradec...	340	C20H36O4	1000309-70-9	53
3	Oxalic acid, cyclobutyl pentadec...	354	C21H38O4	1010309-70-5	52
4	Oxalic acid, cyclobutyl octadecy...	396	C24H44O4	1000309-70-8	46
5	Hexadecane, 1-bromo-	304	C16H33Br	000112-82-3	45





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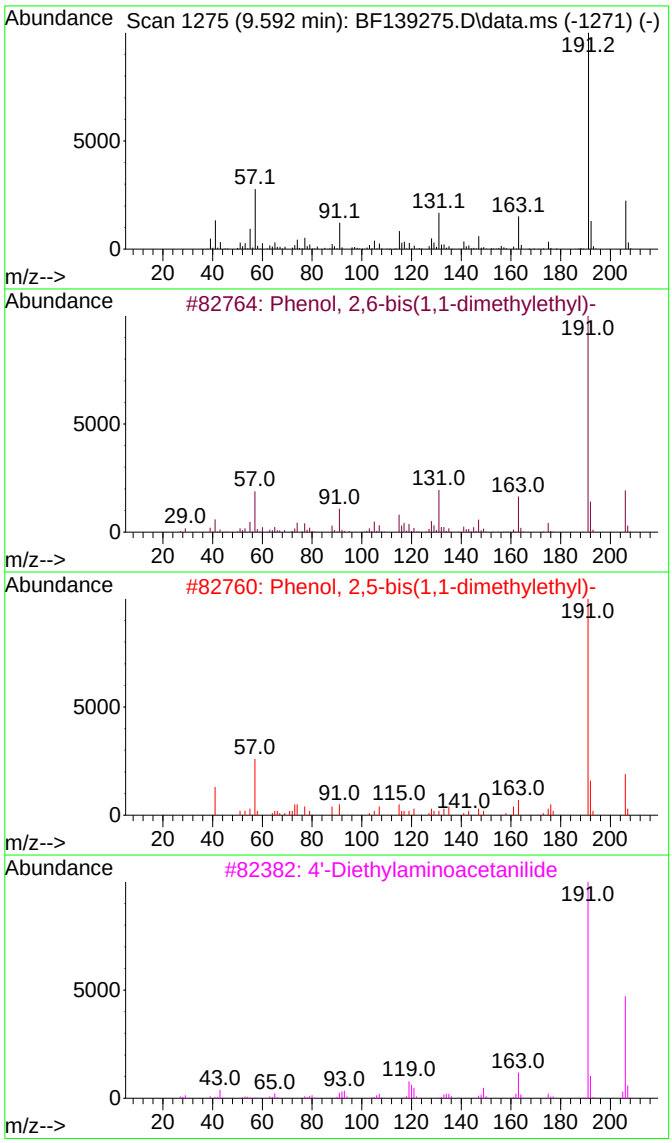
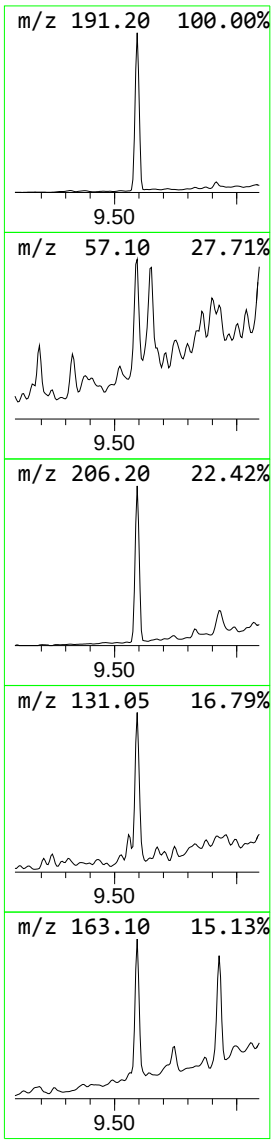
****
Peak Number 8 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.592	19.21 ng	883381	Acenaphthene-d10	9.927

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	96
2	Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	74
3	4'-Diethylaminoacetanilide	206	C12H18N2O	005326-57-8	72
4	Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	72
5	Ethyl 4-t-butylbenzoate	206	C13H18O2	005406-57-5	64





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TIC Library : C:\Database\NIST20.L
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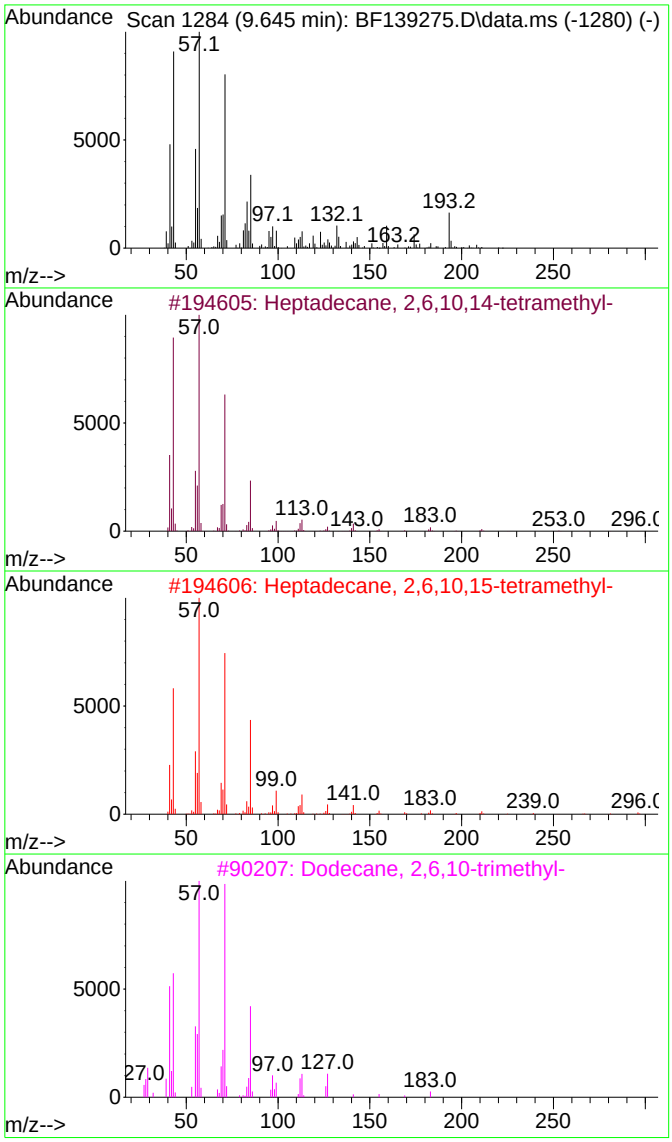
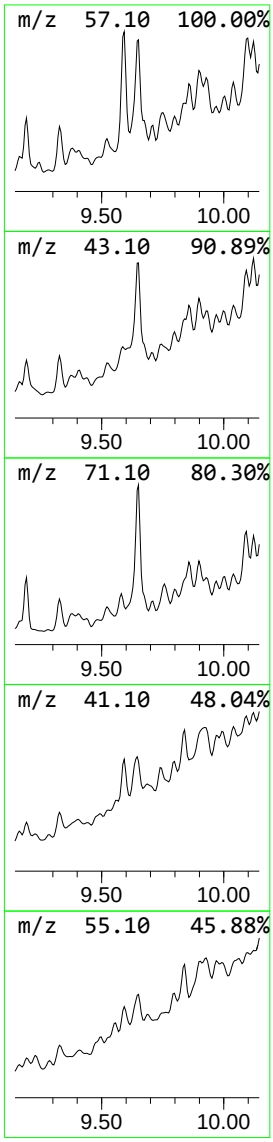
****
Peak Number 9 Heptadecane, 2,6,10,14-tetr... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.645	10.25 ng	471036	Acenaphthene-d10	9.927

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	018344-37-1	58
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	58
3	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	52
4	Tridecane	184	C13H28	000629-50-5	52
5	Butanoic acid, 1-methyloctyl ester	214	C13H26O2	069727-42-0	47





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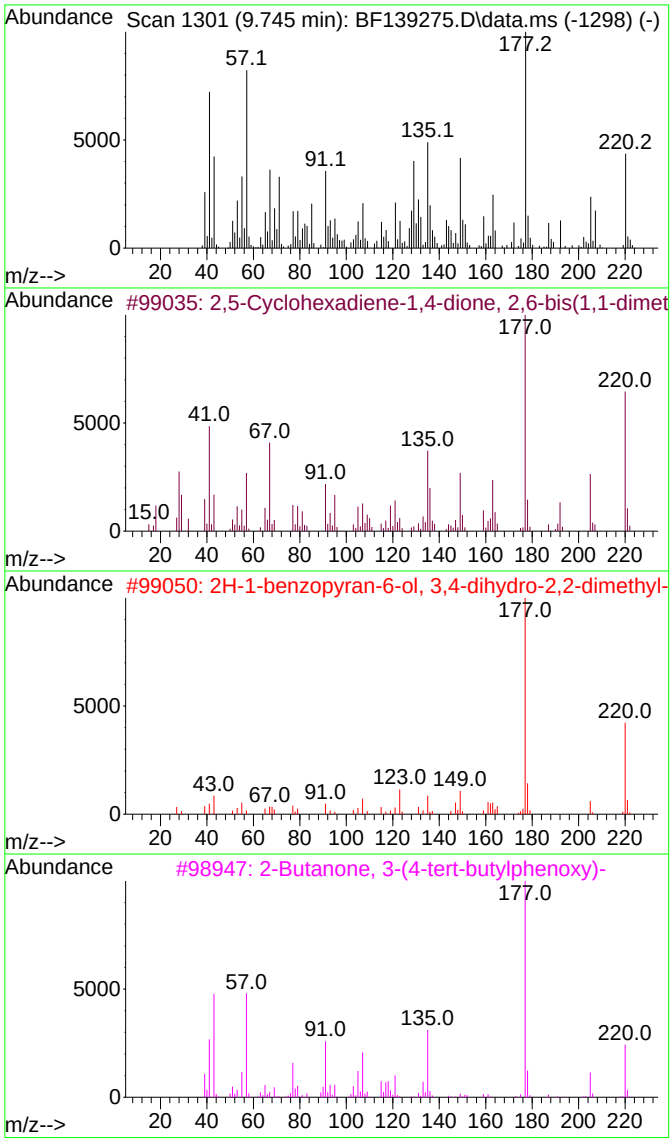
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

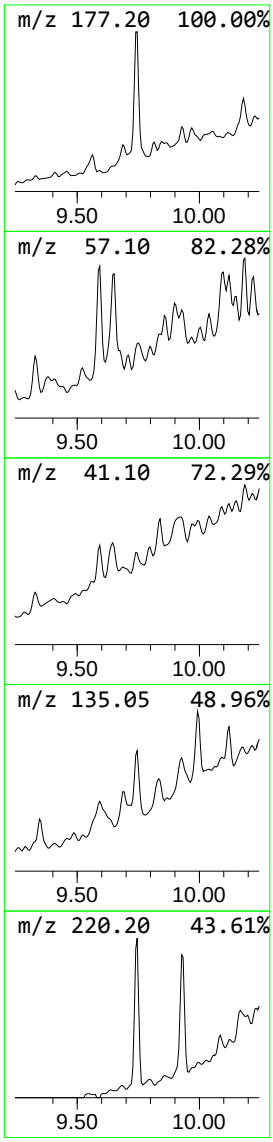
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.745	6.21 ng	285410	Acenaphthene-d10	9.927

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	95
2	2H-1-benzopyran-6-ol, 3,4-dihydr...	220	C14H20O2	1000396-25-4	42
3	2-Butanone, 3-(4-tert-butylpheno...	220	C14H20O2	160875-28-5	41
4	2-Acetyl-3,4,5,6-tetrafluorobenz...	220	C9H4F4O2	1000461-12-2	38
5	3-tert-Butylbenzoic acid, methyl...	192	C12H16O2	027330-57-0	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090624\
Data File : BF139275.D
Acq On : 06 Sep 2024 14:02
Operator : RC/JU
Sample : P3852-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI356

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

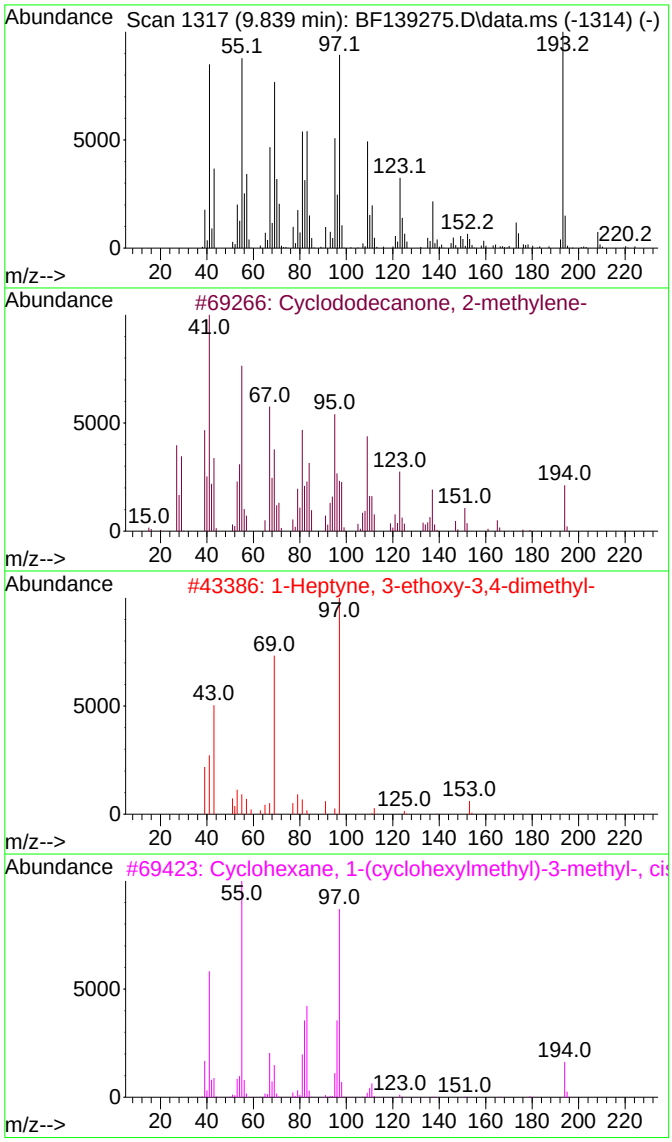
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

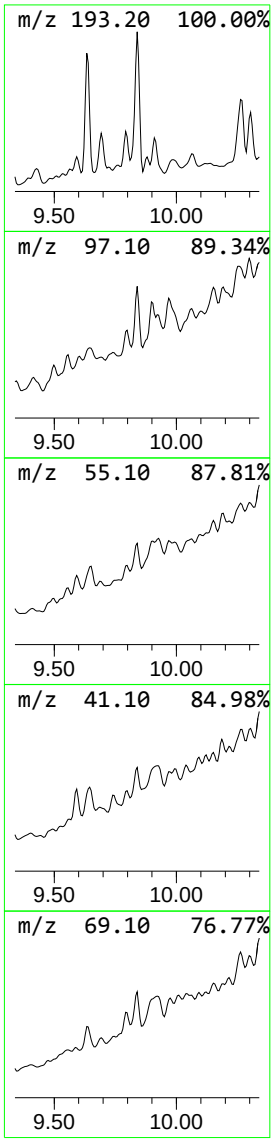
****

Peak Number 11 Cyclododecanone, 2-methylene- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.839	7.02 ng	322553	Acenaphthene-d10	9.927

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	55
2	1-Heptyne, 3-ethoxy-3,4-dimethyl-	168	C11H20O	054411-04-0	27
3	Cyclohexane, 1-(cyclohexylmethyl...	194	C14H26	054823-96-0	18
4	4-Amino-N-hydroxypyrazolo[3,2-c]...	193	C6H7N7O	1000443-50-2	18
5	3a,7a-Epoxy-1H-inden-4(5H)-one, ...	152	C9H12O2	039746-31-1	18





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090624\
Data File : BF139275.D
Acq On : 06 Sep 2024 14:02
Operator : RC/JU
Sample : P3852-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI356

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.128	43.1	ng	1964950	1	6.886	910693	20.0
2-Pentanone, 4-...	5.087	2.9	ng	133353	1	6.886	910693	20.0
1-Hexanol, 2-et...	6.986	3.5	ng	159211	1	6.886	910693	20.0
unknown8.498	8.498	3.4	ng	133087	2	8.169	781775	20.0
unknown8.863	8.863	8.8	ng	342715	2	8.169	781775	20.0
unknown9.057	9.057	6.0	ng	278369	3	9.927	919524	20.0
1-Decanol, 2-he...	9.327	7.7	ng	353025	3	9.927	919524	20.0
Phenol, 2,6-bis...	9.592	19.2	ng	883381	3	9.927	919524	20.0
Heptadecane, 2,...	9.645	10.3	ng	471036	3	9.927	919524	20.0
2,5-Cyclohexadi...	9.745	6.2	ng	285410	3	9.927	919524	20.0
Cyclododecanone...	9.839	7.0	ng	322553	3	9.927	919524	20.0