LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090924\
Data File : BF139287.D
Acq On : 09 Sep 2024 17:18
Operator : RC/JU
Sample : P3892-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ARS20-005

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: BF139287.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	7	14	rVB	1809419	2730649	100.00%	16.445%
2	5.092	501	510	517	rVB	136955	211754	7.75%	1.275%
3	5.498	573	579	584	rBV	1656025	2162346	79.19%	13.023%
4	6.510	745	751	756	rBV	1676602	2232714	81.76%	13.447%
5	6.886	810	815	820	rBV	521019	628609	23.02%	3.786%
6	7.445	901	910	915	rBV	1074110	1426665	52.25%	8.592%
7	8.075	1013	1017	1021	rVB2	124457	154101	5.64%	0.928%
8	8.169	1027	1033	1037	rBV	612265	855423	31.33%	5.152%
9	8.228	1040	1043	1046	rVB2	130288	162611	5.96%	0.979%
10	8.275	1046	1051	1055	rBV6	94245	224387	8.22%	1.351%
11	8.345	1060	1063	1066	rBV2	139468	197432	7.23%	1.189%
12	8.463	1079	1083	1086	rBV2	216324	313252	11.47%	1.887%
13	8.557	1096	1099	1101	rBV2	147589	198834	7.28%	1.197%
14	8.798	1137	1140	1143	rBV	202436	282735	10.35%	1.703%
15	9.198	1206	1208	1211	rVB	526591	524739	19.22%	3.160%
16	9.251	1212	1217	1220	rBV2	1562876	2301873	84.30%	13.863%
17	15.551	2285	2288	2308	rVB	284429	702402	25.72%	4.230%
18	17.633	2635	2642	2651	rBV3	95553	262246	9.60%	1.579%
19	18.215	2734	2741	2751	rVB4	131475	422755	15.48%	2.546%
20	18.456	2774	2782	2800	rVB3	191796	608893	22.30%	3.667%

Sum of corrected areas: 16604420

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090924\
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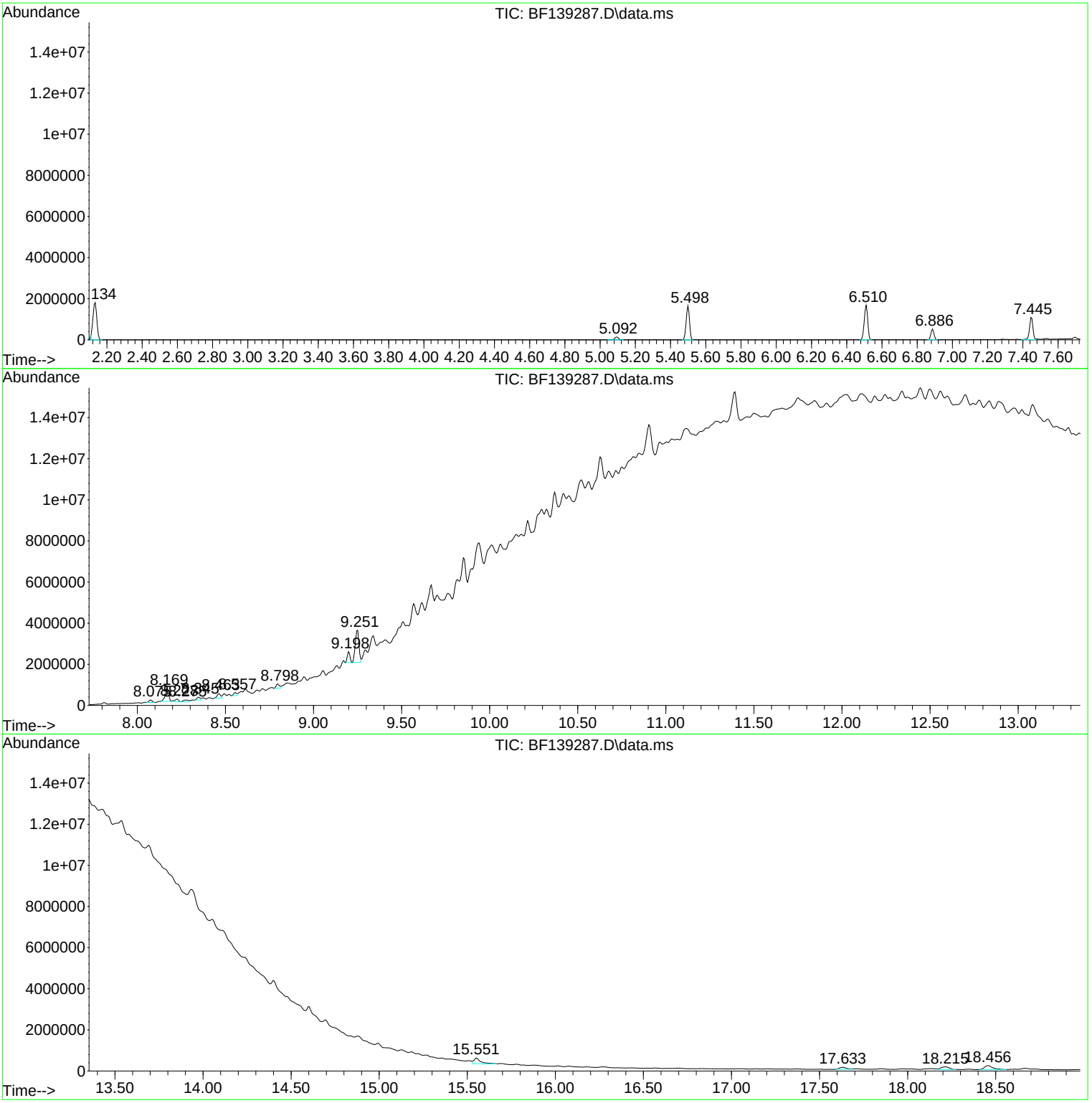
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ARS20-005

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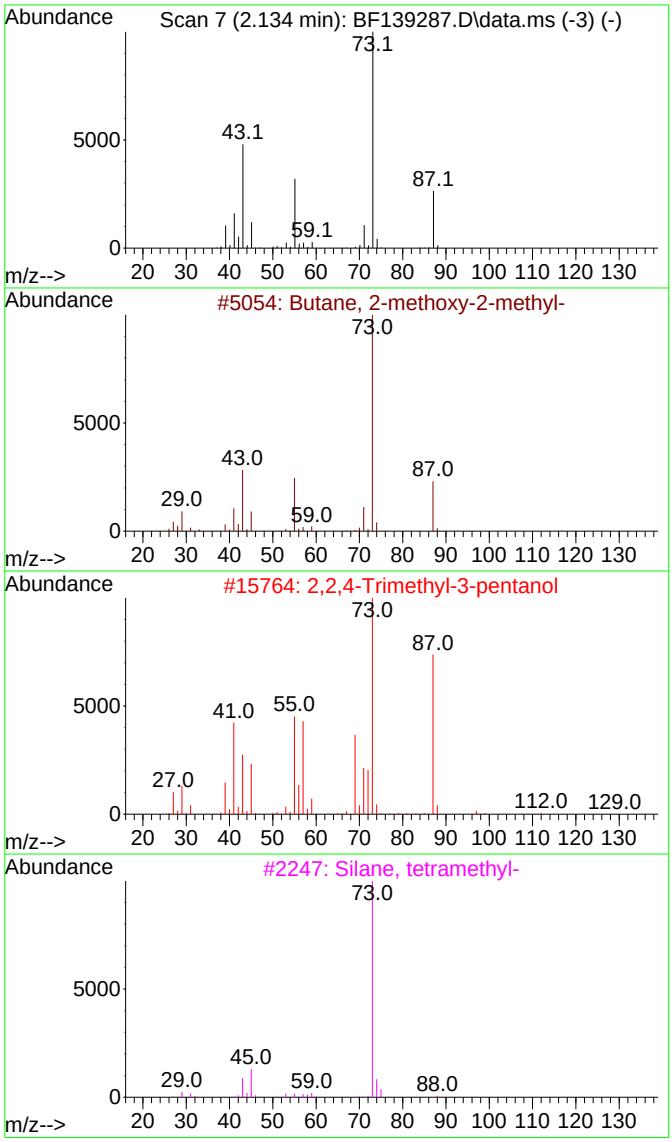
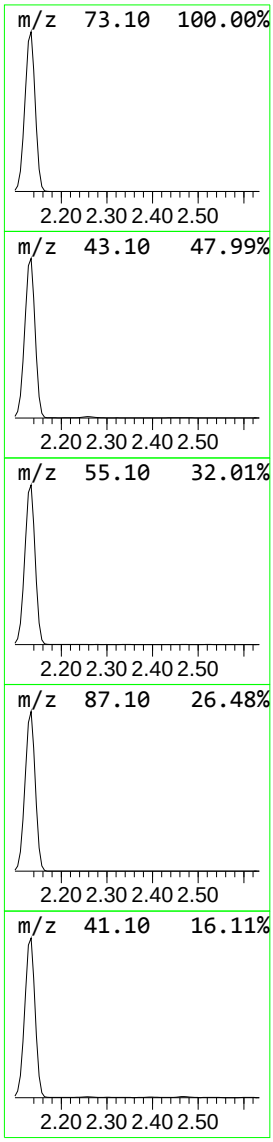
****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	86.88 ng	2730650	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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





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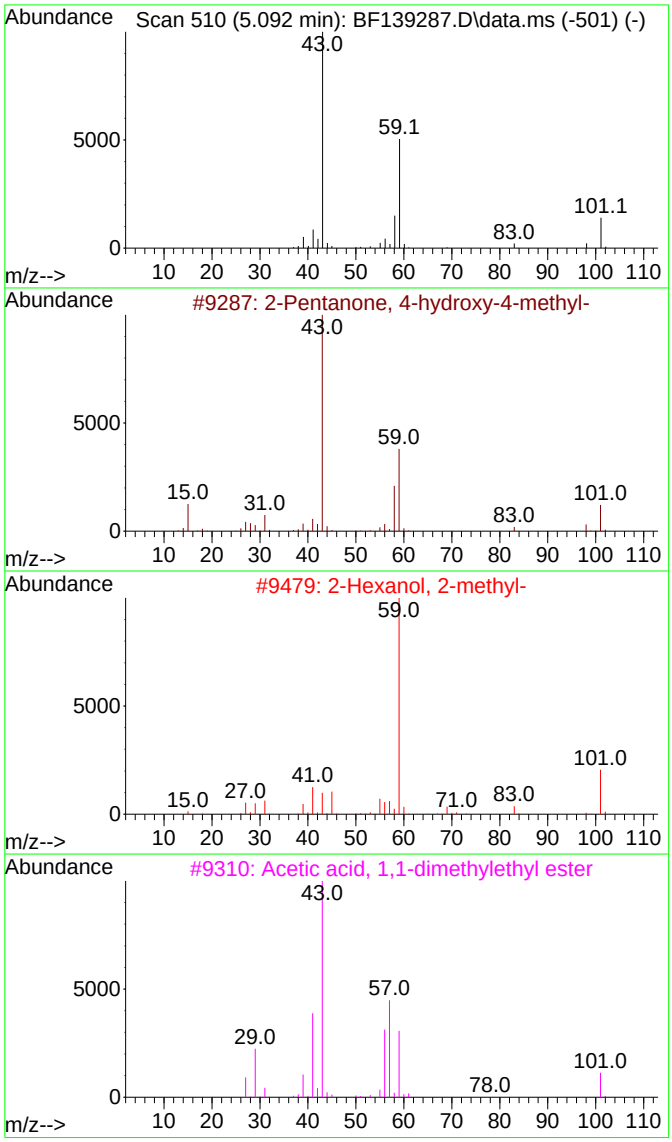
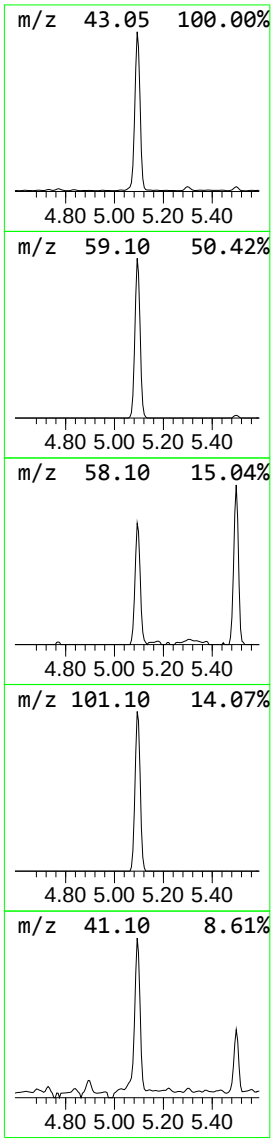
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.092	6.74 ng	211754	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-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
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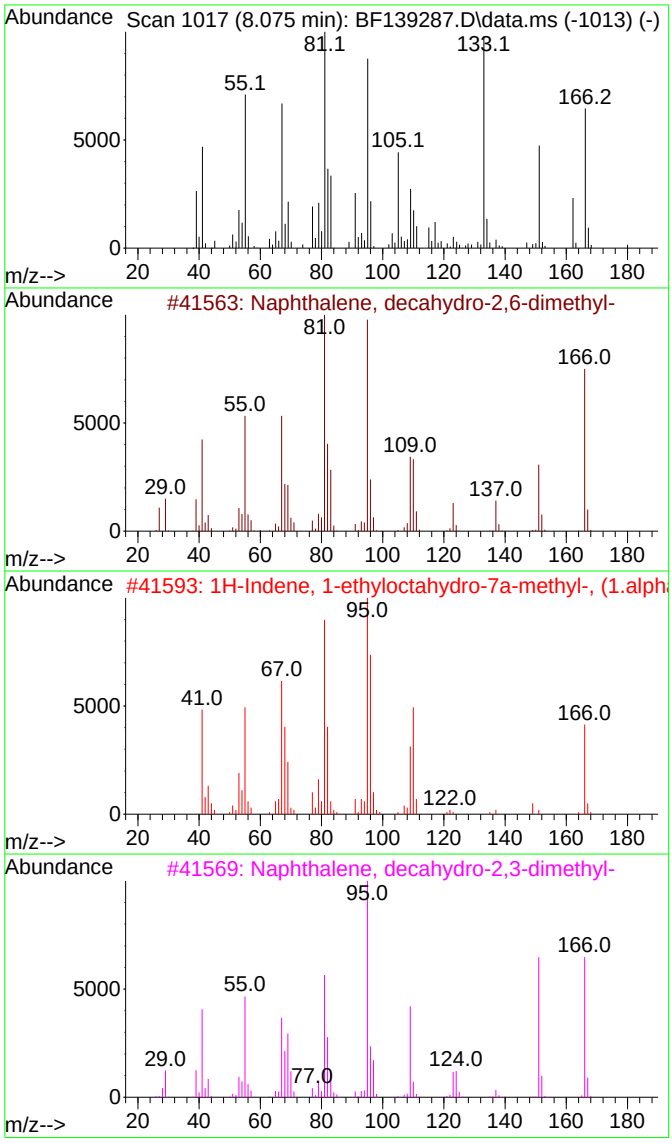
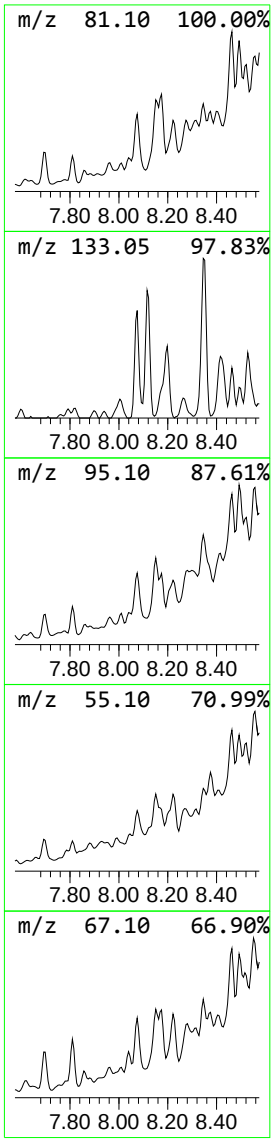
****
Peak Number 3 Naphthalene, decahydro-2,6-... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.075	3.60 ng	154101	Naphthalene-d8	8.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-2,6-dimet...	166	C12H22	001618-22-0	86
2	1H-Indene, 1-ethyloctahydro-7a-m...	166	C12H22	056324-71-1	53
3	Naphthalene, decahydro-2,3-dimet...	166	C12H22	001008-80-6	49
4	cis,trans-1,6-Dimethylspiro[4.5]...	166	C12H22	1000111-72-3	47
5	Cyclohexene,1-hexyl-	166	C12H22	003964-66-7	38





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
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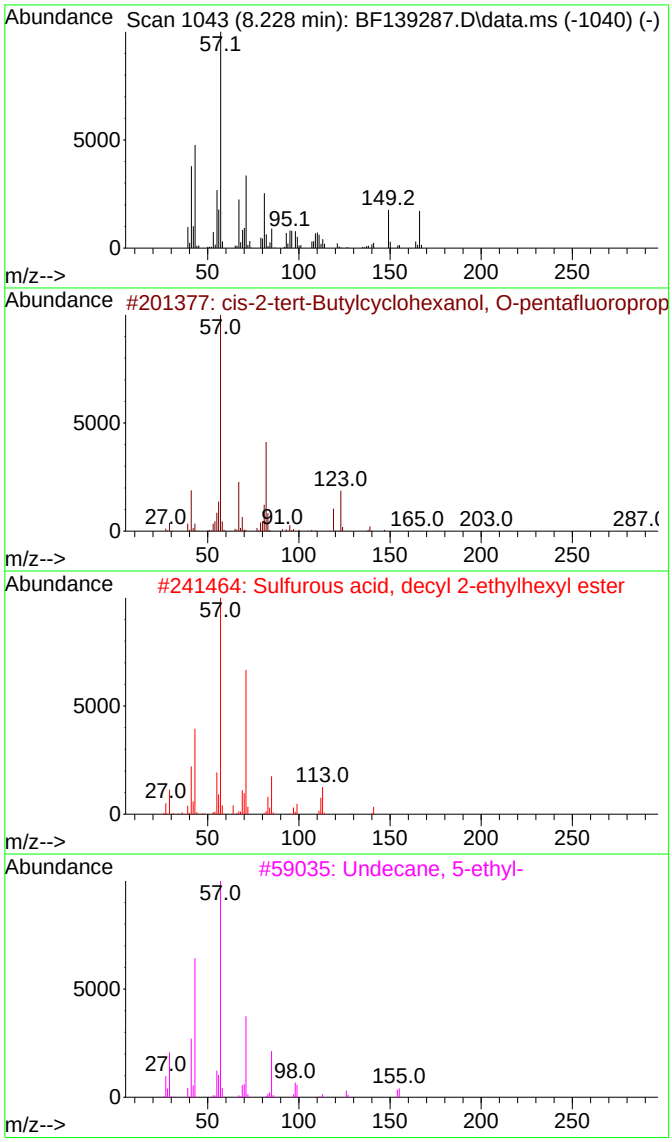
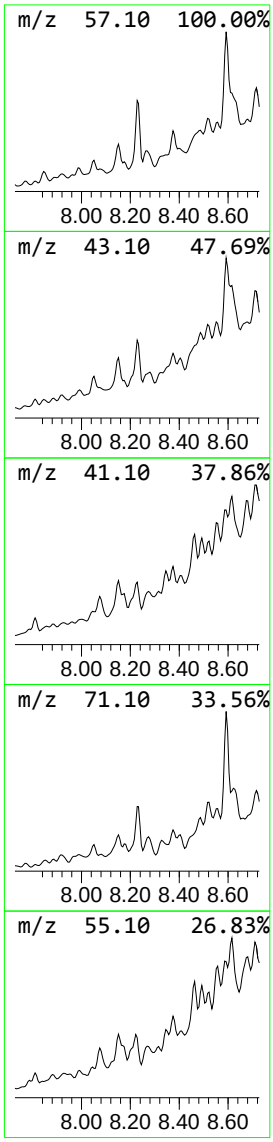
****

Peak Number 4 unknown8.228 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.228	3.80 ng	162611	Naphthalene-d8	8.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-2-tert-Butylcyclohexanol, O-...	302	C13H19F5O2	1000467-24-6	27
2	Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	27
3	Undecane, 5-ethyl-	184	C13H28	017453-94-0	27
4	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	27
5	Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	27





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
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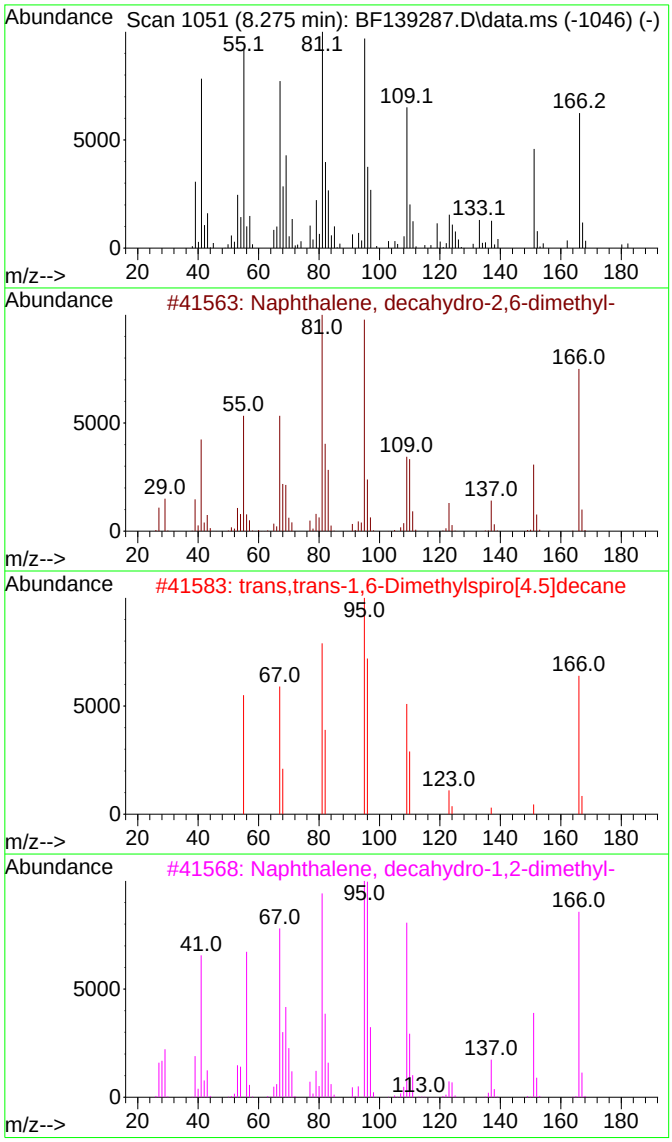
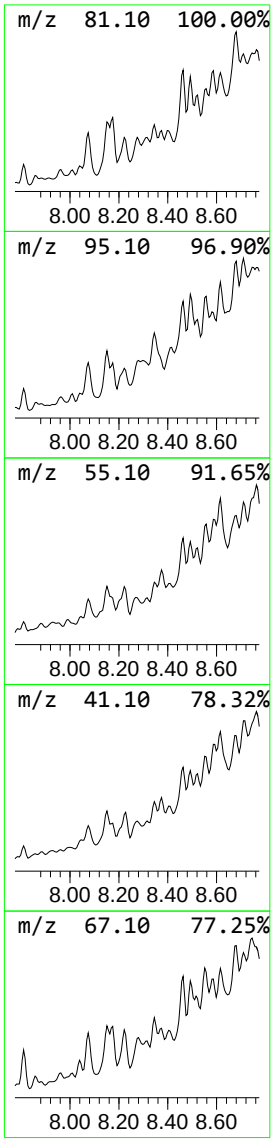
****
Peak Number 5 trans,trans-1,6-Dimethylspi... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.275	5.25 ng	224387	Naphthalene-d8	8.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-2,6-dimet...	166	C12H22	001618-22-0	90
2	trans,trans-1,6-Dimethylspiro[4....	166	C12H22	1000111-72-1	90
3	Naphthalene, decahydro-1,2-dimet...	166	C12H22	003604-14-6	89
4	cis,cis-1,6-Dimethylspiro[4.5]de...	166	C12H22	1000111-72-4	81
5	cis,trans-1,6-Dimethylspiro[4.5]...	166	C12H22	1000111-72-3	76





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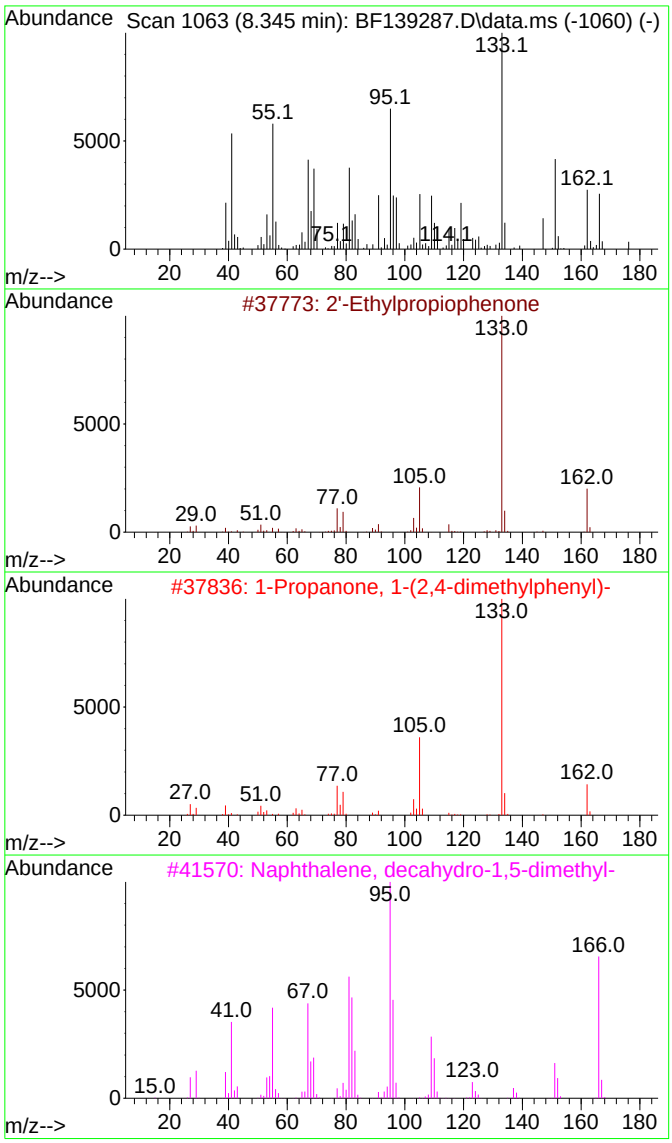
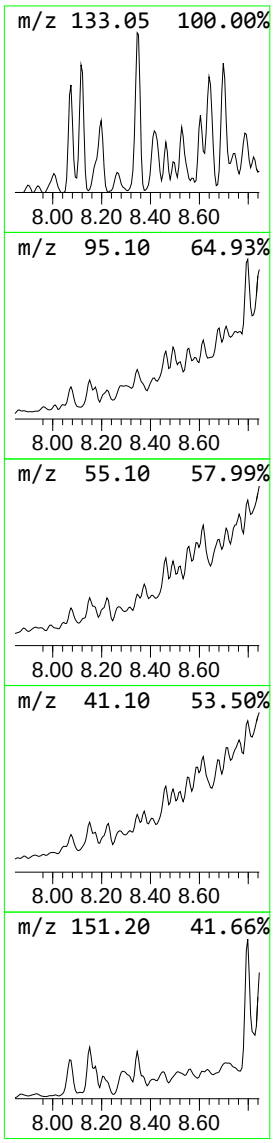
****

Peak Number 6 unknown8.345 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.345	4.62 ng	197432	Naphthalene-d8	8.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2'-Ethylpropiophenone	162	C11H14O	016819-79-7	35
2	1-Propanone, 1-(2,4-dimethylphen...	162	C11H14O	035031-55-1	35
3	Naphthalene, decahydro-1,5-dimet...	166	C12H22	066552-62-3	30
4	2-Amino-6-methylbenzoic acid	151	C8H9NO2	004389-50-8	25
5	cis,cis-1,6-Dimethylspiro[4.5]de...	166	C12H22	1000111-72-4	25





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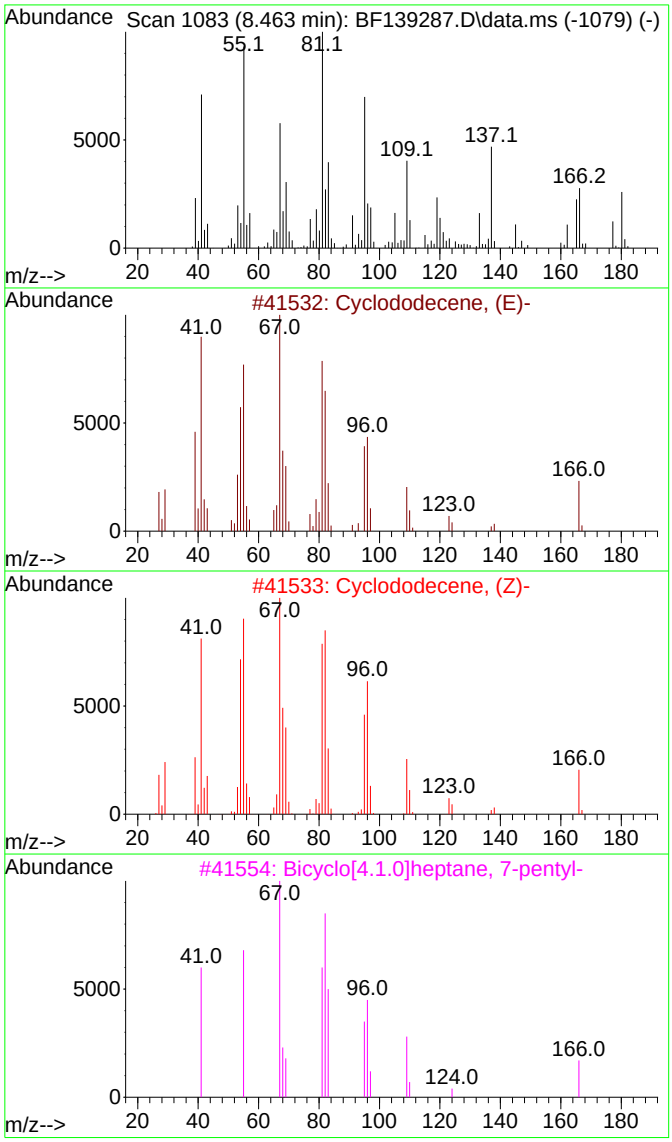
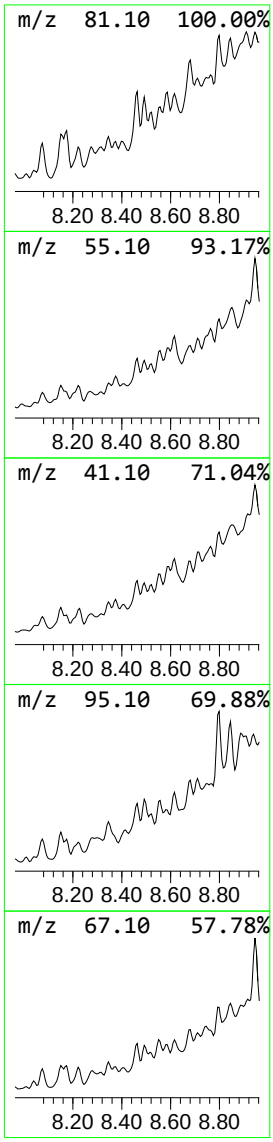
****

Peak Number 7 unknown8.463 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.463	7.32 ng	313252	Naphthalene-d8	8.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclododecene, (E)-	166	C12H22	001486-75-5	49
2	Cyclododecene, (Z)-	166	C12H22	001129-89-1	46
3	Bicyclo[4.1.0]heptane, 7-pentyl-	166	C12H22	041977-45-1	45
4	trans,cis-2,8-Dimethylspiro[5.5]...	180	C13H24	095472-52-9	43
5	cis,trans-2,9-Dimethylspiro[5.5]...	180	C13H24	095530-74-8	43





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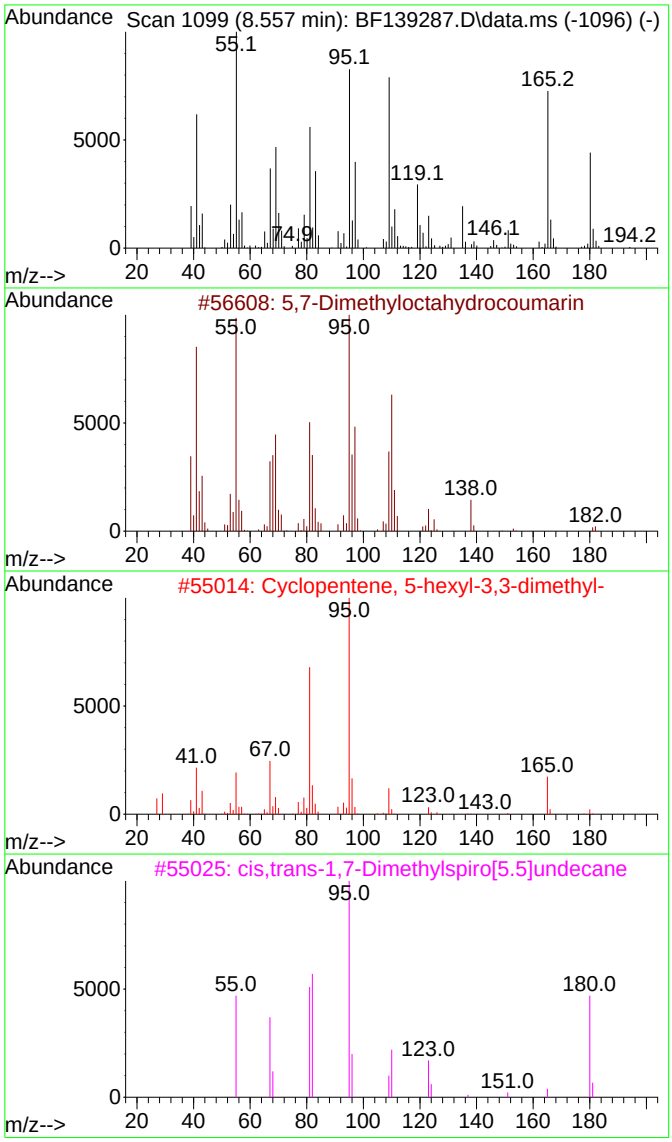
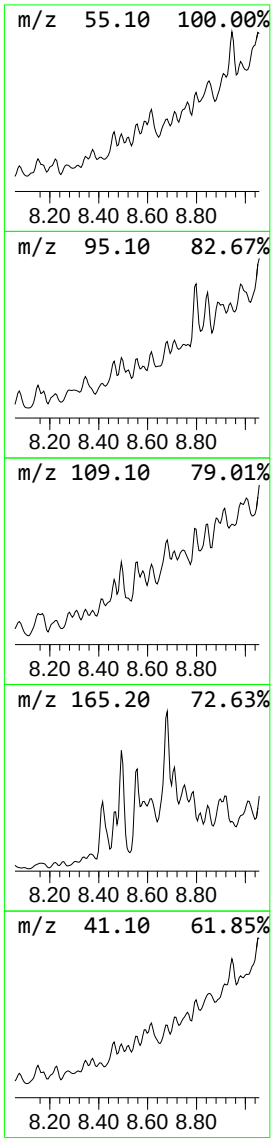
****

Peak Number 8 unknown8.557 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.557	4.65 ng	198834	Naphthalene-d8	8.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,7-Dimethyloctahydrocoumarin	182	C11H18O2	1000109-81-5	38
2	Cyclopentene, 5-hexyl-3,3-dimethyl-	180	C13H24	061142-66-3	35
3	cis,trans-1,7-Dimethylspiro[5.5]...	180	C13H24	1000111-73-1	30
4	4-Methyl-4-(1H-pyrazol-5-yl)pipe...	165	C9H15N3	1000460-41-6	25
5	4-Methoxypyridine-2-carboxamide,...	180	C9H12N2O2	1872090-67-9	22





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TIC Library : C:\Database\NIST20.L
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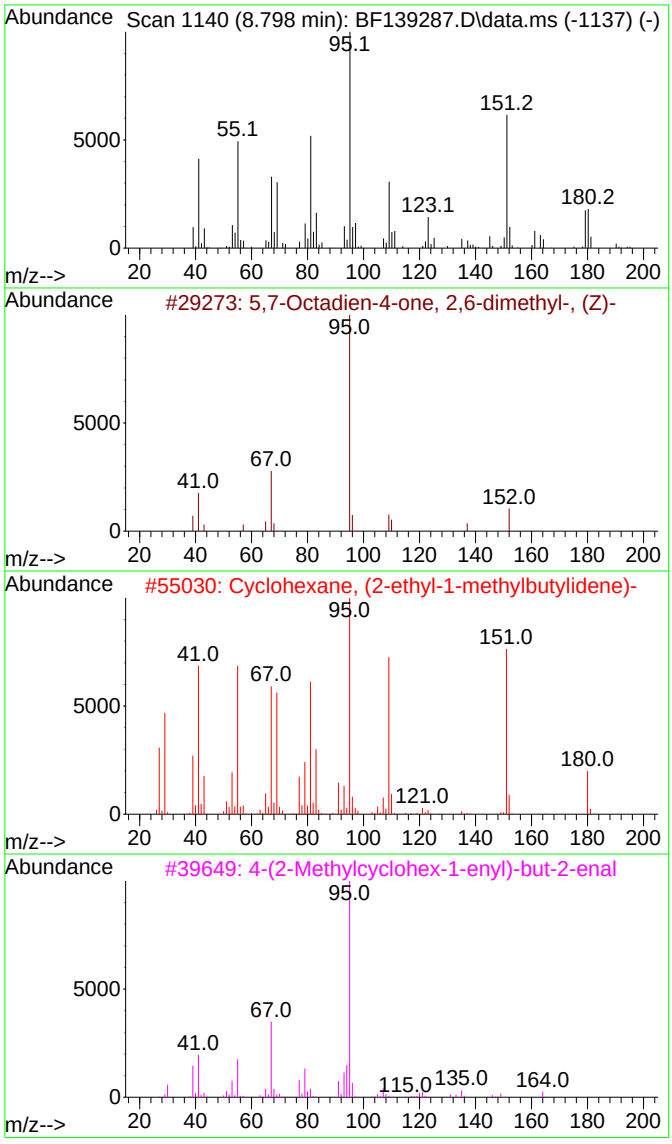
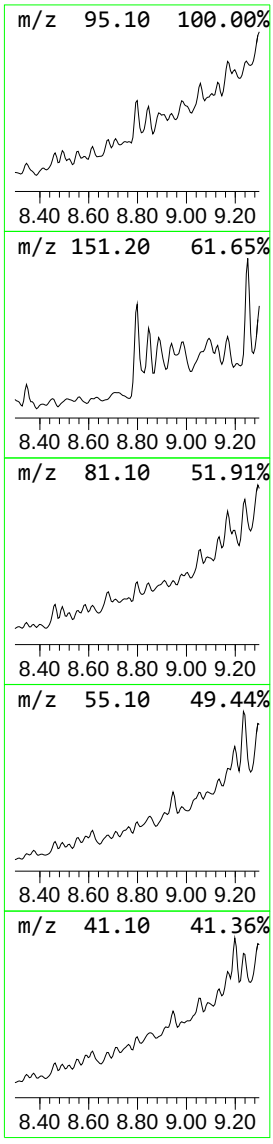
Peak Number 9 unknown8.798 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.798	6.61 ng	282735	Naphthalene-d8	8.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	003588-18-9	46
2	Cyclohexane, (2-ethyl-1-methylbu...	180	C13H24	074810-41-6	46
3	4-(2-Methylcyclohex-1-enyl)-but-...	164	C11H16O	1000188-10-0	43
4	4-Methyl-1,3-heptadiene	110	C8H14	017603-57-5	38
5	2-Furancarboxamide, N-methyl-	125	C6H7NO2	1010407-23-7	38





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
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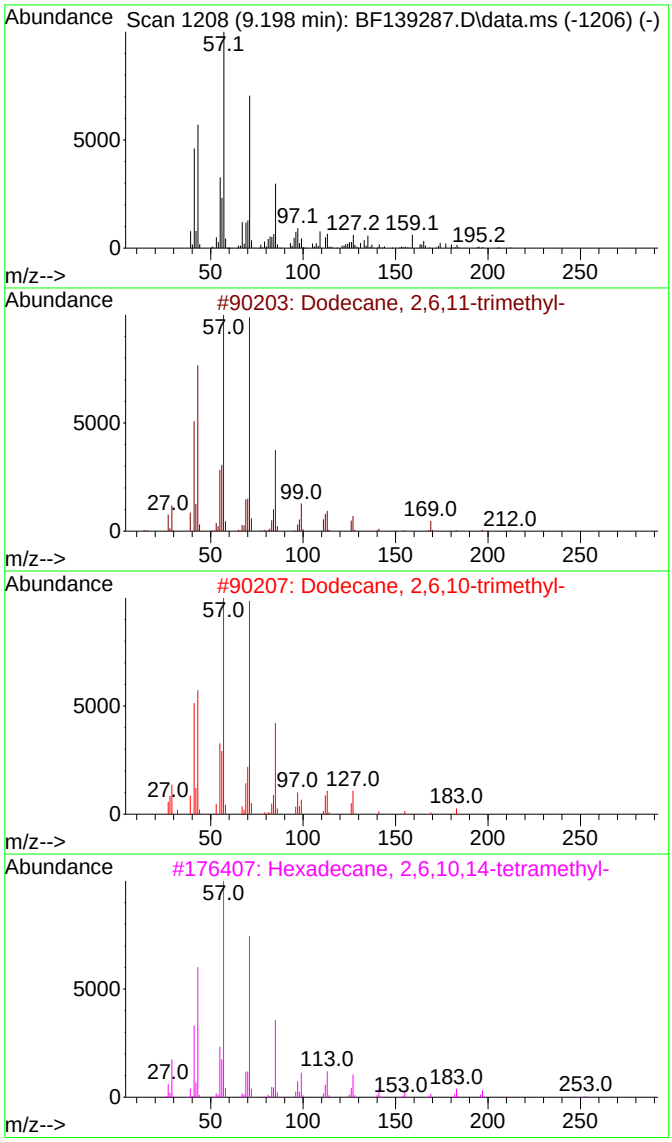
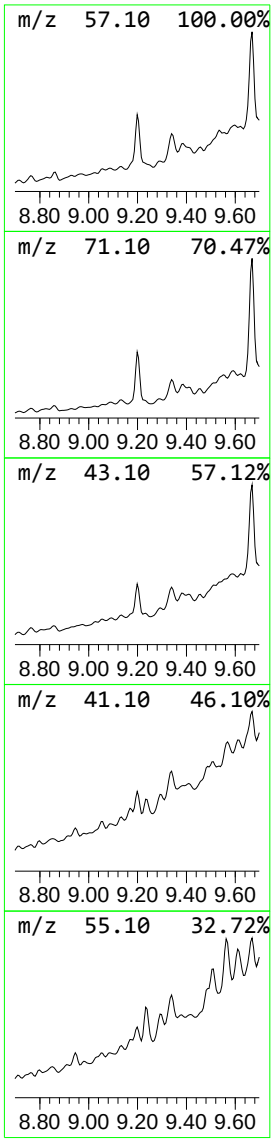
****
Peak Number 10 Dodecane, 2,6,11-trimethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.198	4.56 ng	524739	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	89
2	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	74
3	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	72
4	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	72
5	Octane, 2-methyl-	128	C9H20	003221-61-2	64





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Acq On : 09 Sep 2024 17:18
Operator : RC/JU
Sample : P3892-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ARS20-005

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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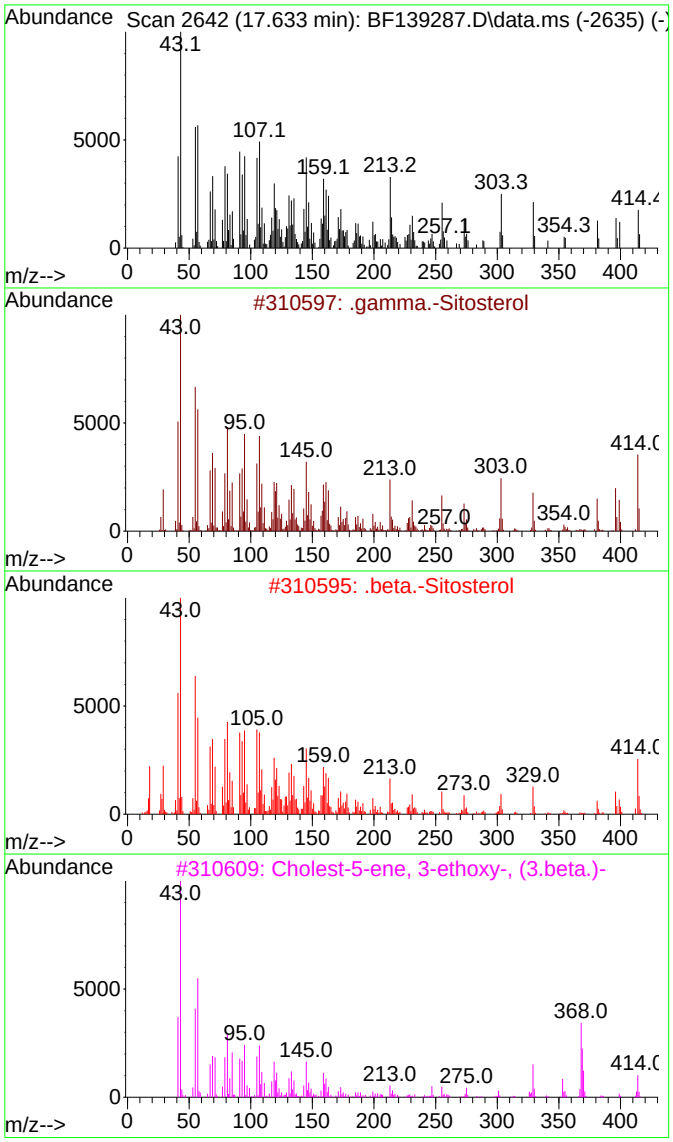
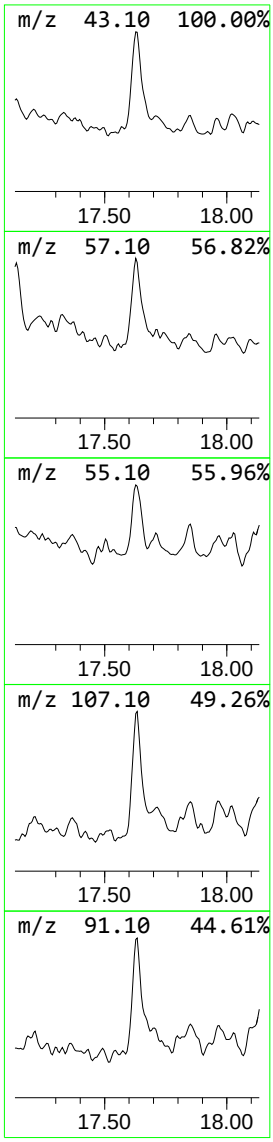
Peak Number 11 .gamma.-Sitosterol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.633	7.47 ng	262246	Perylene-d12	15.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	98
3	Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	70
4	Stigmasta-3,5-diene	396	C29H48	004970-37-0	38
5	Stigmastan-3-en-6-ol	414	C29H50O	1000214-19-7	25





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Acq On : 09 Sep 2024 17:18
Operator : RC/JU
Sample : P3892-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ARS20-005

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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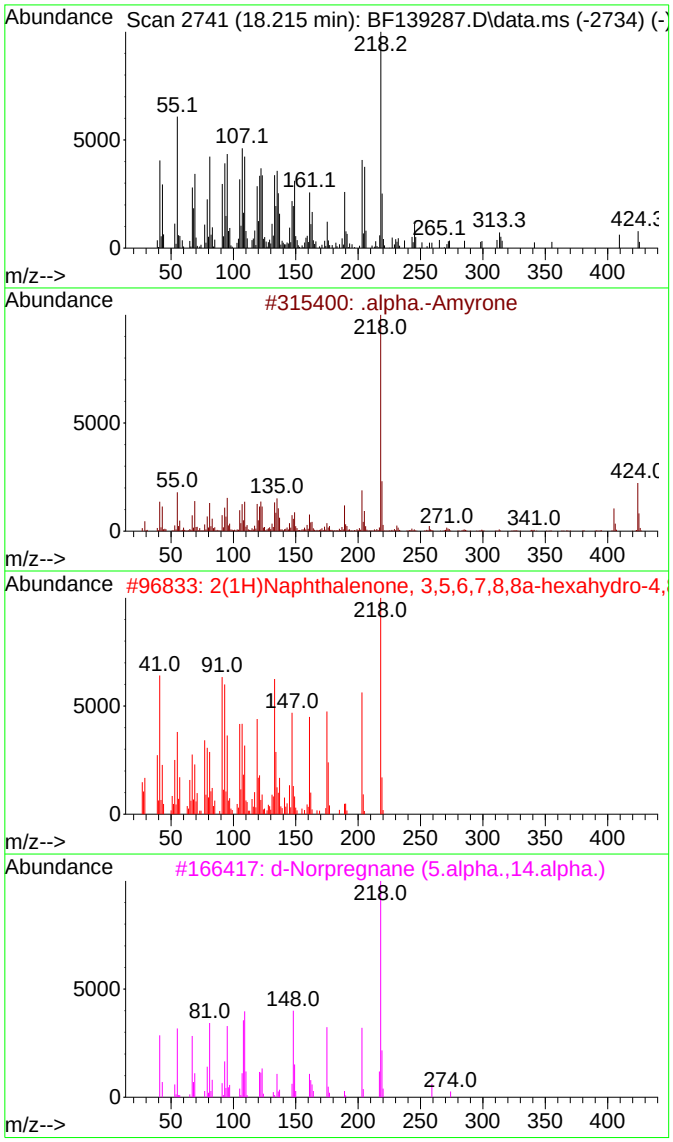
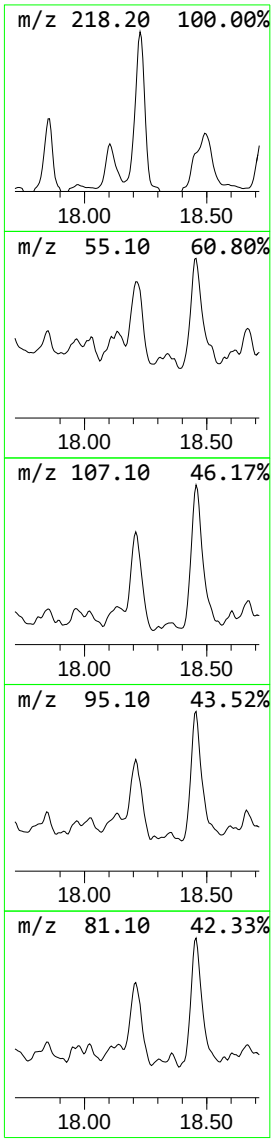
Peak Number 12 .alpha.-Amyrone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.215	12.04 ng	422755	Perylene-d12	15.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Amyrone	424	C30H48O	000638-96-0	98
2	2(1H)Naphthalenone, 3,5,6,7,8,8a...	218	C15H22O	1000188-66-5	78
3	d-Norpregnane (5.alpha.,14.alpha.)	274	C20H34	1000281-13-7	59
4	(1S,6R,9S)-5,5,9,10-Tetramethylt...	218	C16H26	1000298-97-8	52
5	(Z)-2-((8R,8aS)-8,8a-Dimethyl-3,...	218	C15H22O	137695-20-6	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090924\
Data File : BF139287.D
Acq On : 09 Sep 2024 17:18
Operator : RC/JU
Sample : P3892-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ARS20-005

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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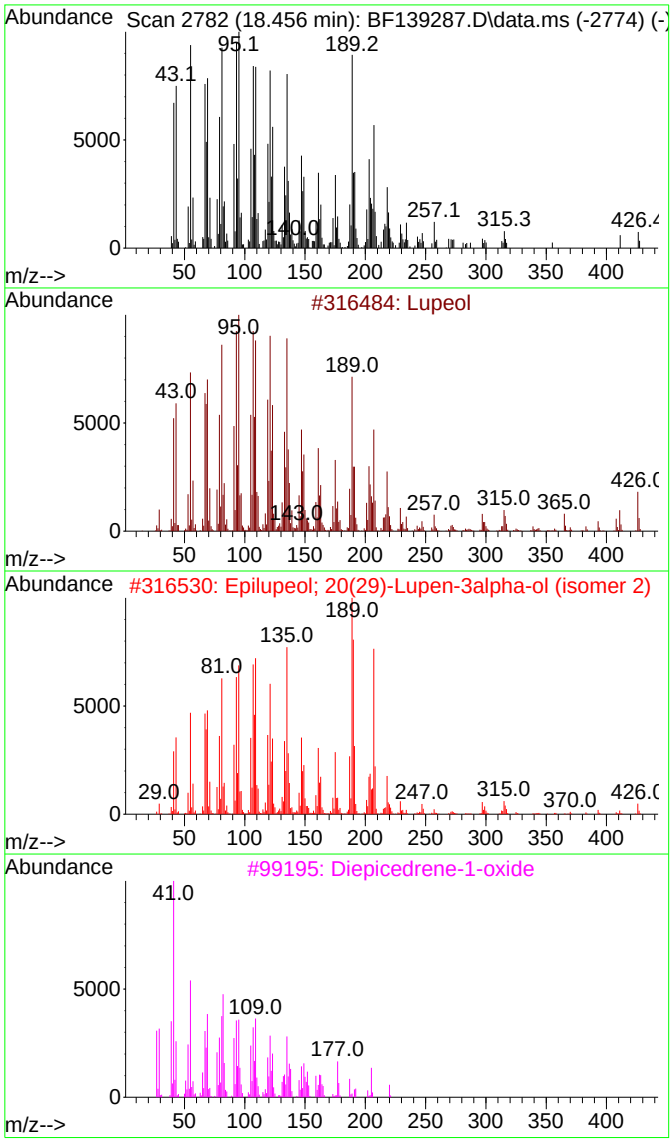
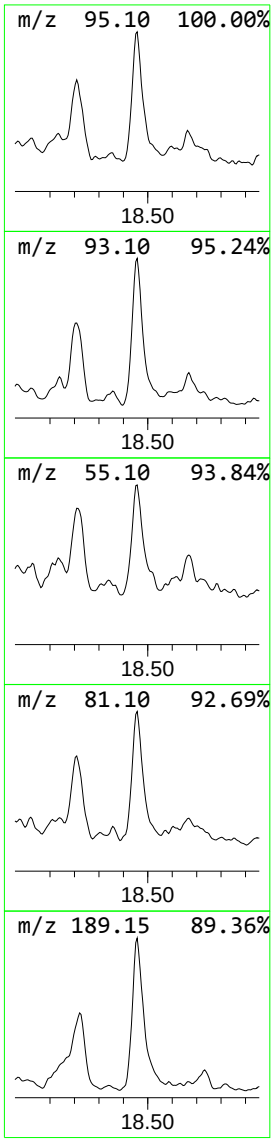
Peak Number 13 Lupeol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.456	17.34 ng	608893	Perylene-d12	15.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lupeol	426	C30H50O	000545-47-1	99
2	Epilupeol; 20(29)-Lupen-3alpha-o...	426	C30H50O	1000513-01-4	87
3	Diepicedrene-1-oxide	220	C15H24O	1000156-11-0	70
4	(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	70
5	Epilupeol; 20(29)-Lupen-3alpha-o...	426	C30H50O	1000513-01-3	70





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090924\
Data File : BF139287.D
Acq On : 09 Sep 2024 17:18
Operator : RC/JU
Sample : P3892-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ARS20-005

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...	2.134	86.9	ng	2730650	1	6.886	628609	20.0
2-Pentanone, 4-...	5.092	6.7	ng	211754	1	6.886	628609	20.0
Naphthalene, de...	8.075	3.6	ng	154101	2	8.169	855423	20.0
unknown8.228	8.228	3.8	ng	162611	2	8.169	855423	20.0
trans,trans-1,6...	8.275	5.3	ng	224387	2	8.169	855423	20.0
unknown8.345	8.345	4.6	ng	197432	2	8.169	855423	20.0
unknown8.463	8.463	7.3	ng	313252	2	8.169	855423	20.0
unknown8.557	8.557	4.7	ng	198834	2	8.169	855423	20.0
unknown8.798	8.798	6.6	ng	282735	2	8.169	855423	20.0
Dodecane, 2,6,1...	9.198	4.6	ng	524739	3	9.939	2301870	20.0
.gamma.-Sitosterol	17.633	7.5	ng	262246	6	15.551	702402	20.0
.alpha.-Amyrone	18.215	12.0	ng	422755	6	15.551	702402	20.0
Lupeol	18.456	17.3	ng	608893	6	15.551	702402	20.0