LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091824\
Data File : BF139437.D
Acq On : 18 Sep 2024 20:44
Operator : RC/JU
Sample : P4023-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONCRETE-TP-9

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-BF091324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139437.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	8	16	24	rVB	817804	1308147	75.37%	10.269%
2	4.481	399	406	412	rBV	603084	862594	49.70%	6.771%
3	5.093	501	510	521	rVB	483737	710429	40.93%	5.577%
4	5.499	573	579	584	rBV	847683	1099366	63.34%	8.630%
5	6.504	744	750	755	rBV	1096922	1469048	84.64%	11.532%
6	6.875	808	813	818	rVB	343255	416502	24.00%	3.269%
7	7.193	863	867	872	rBV	20847	26001	1.50%	0.204%
8	7.440	903	909	914	rBV	812897	1043122	60.10%	8.188%
9	7.693	947	952	959	rVB	19564	24448	1.41%	0.192%
10	8.157	1026	1031	1036	rBV	419249	503144	28.99%	3.950%
11	9.234	1208	1214	1219	rBV	1395322	1735634	100.00%	13.625%
12	9.910	1324	1329	1334	rBV	397096	484240	27.90%	3.801%
13	10.622	1445	1450	1457	rBV	63895	80198	4.62%	0.630%
14	10.692	1457	1462	1475	rVV	382634	495989	28.58%	3.893%
15	11.392	1576	1581	1587	rBV	327093	405127	23.34%	3.180%
16	11.916	1665	1670	1681	rBV2	31078	51492	2.97%	0.404%
17	12.980	1845	1851	1856	rBV	947978	1257098	72.43%	9.868%
18	13.874	1998	2003	2015	rBV	53306	115026	6.63%	0.903%
19	14.027	2024	2029	2037	rVB	265831	347107	20.00%	2.725%
20	15.498	2274	2279	2289	rVB	162871	273331	15.75%	2.146%
21	15.645	2301	2304	2312	rVB9	18169	30987	1.79%	0.243%

Sum of corrected areas: 12739030

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091824\
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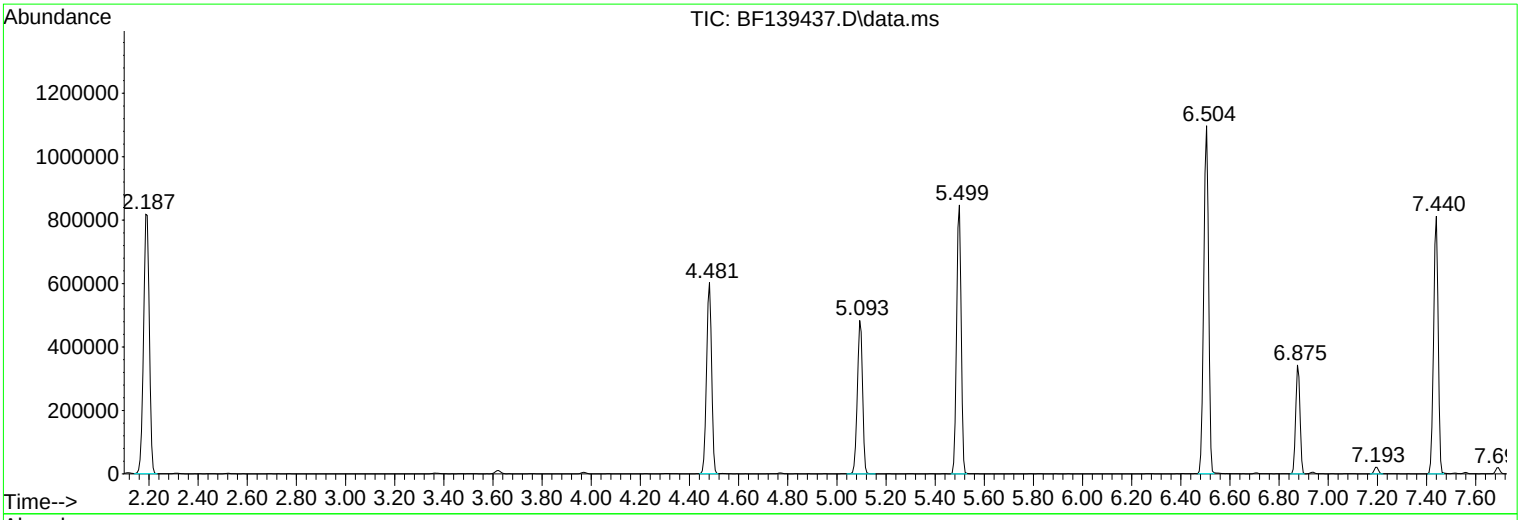
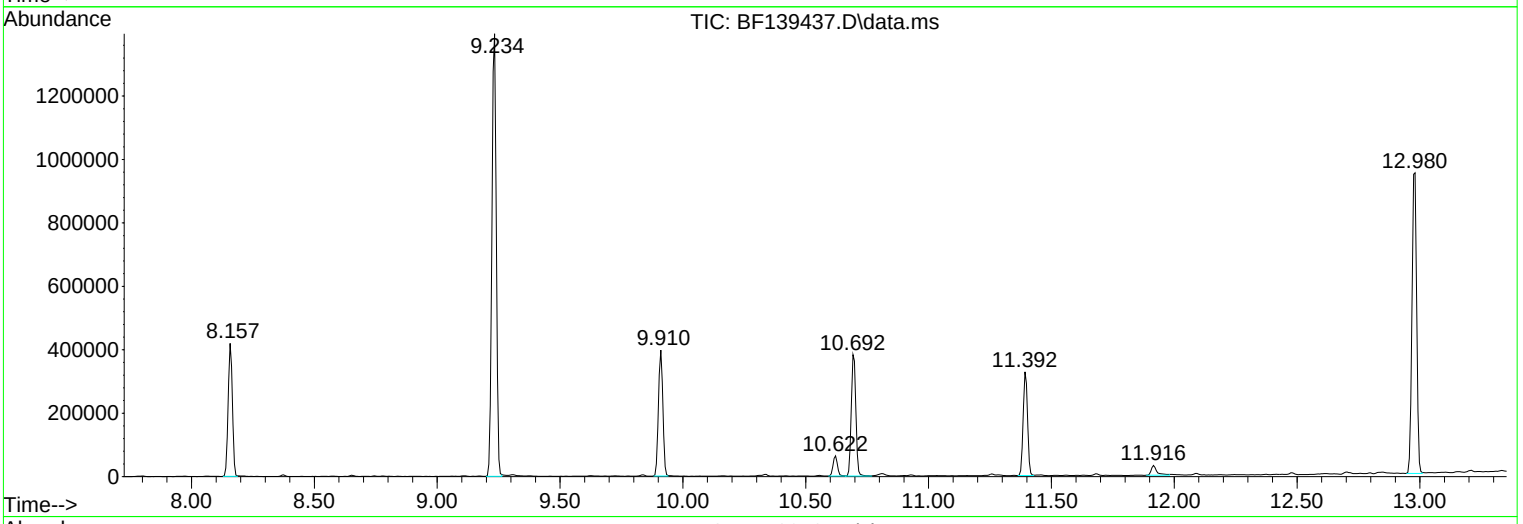
Misc :
ALS Vial : 11 Sample Multiplier: 1

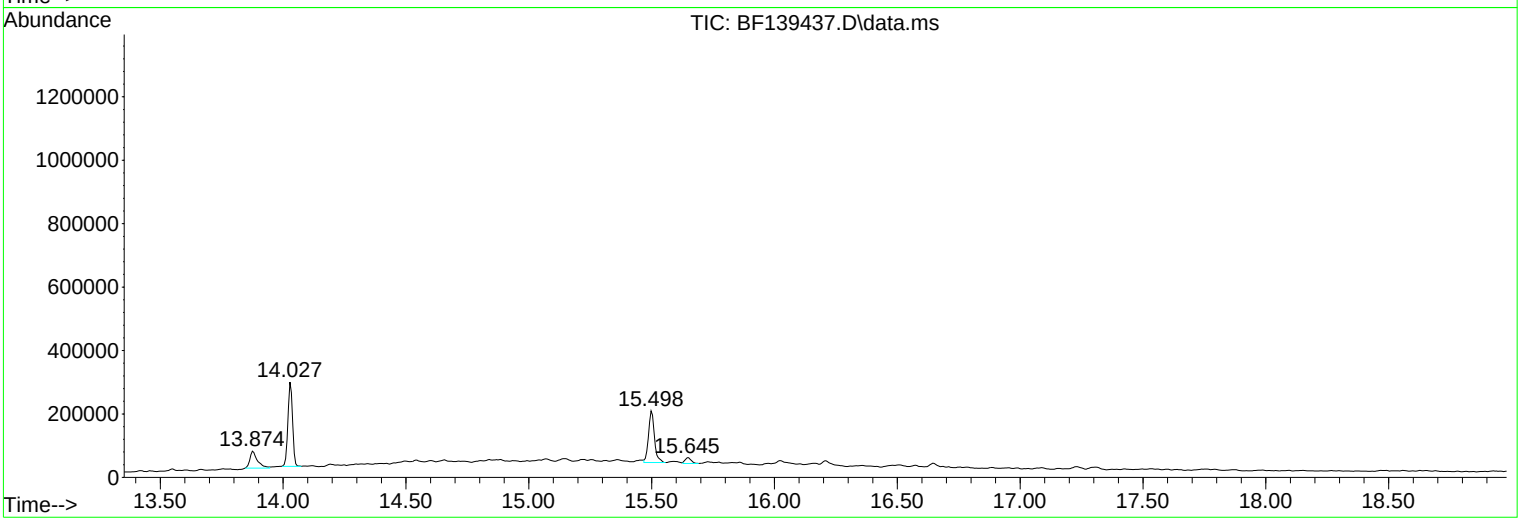
Instrument :
BNA_F
ClientSampleId :
CONCRETE-TP-9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.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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Data File : BF139437.D
Acq On : 18 Sep 2024 20:44
Operator : RC/JU
Sample : P4023-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONCRETE-TP-9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

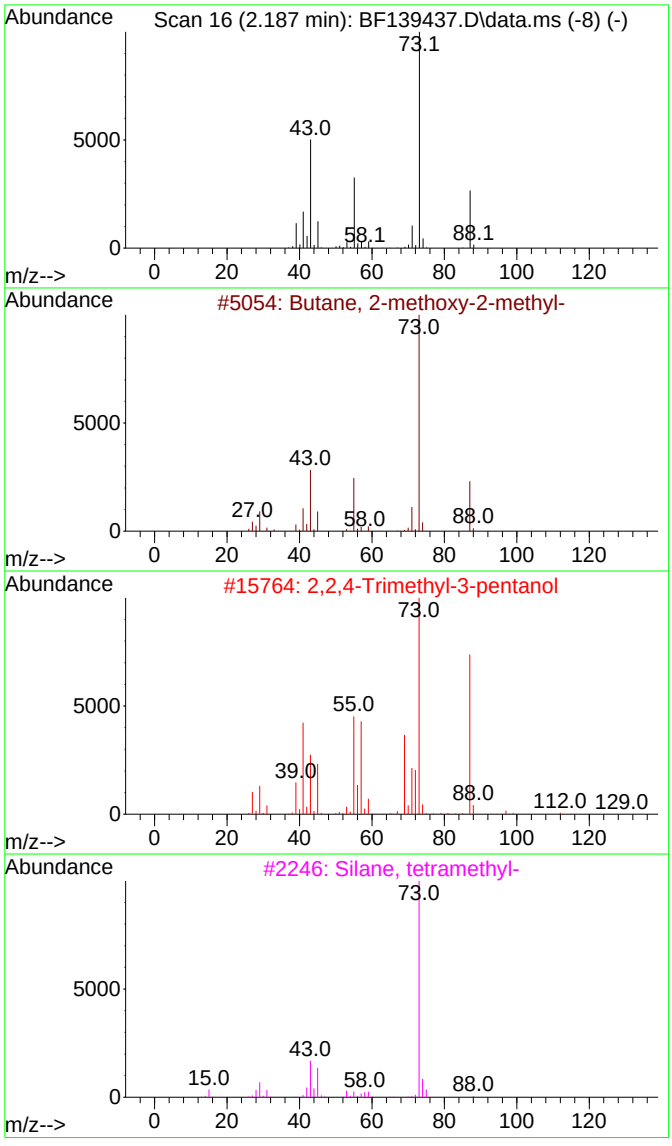
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

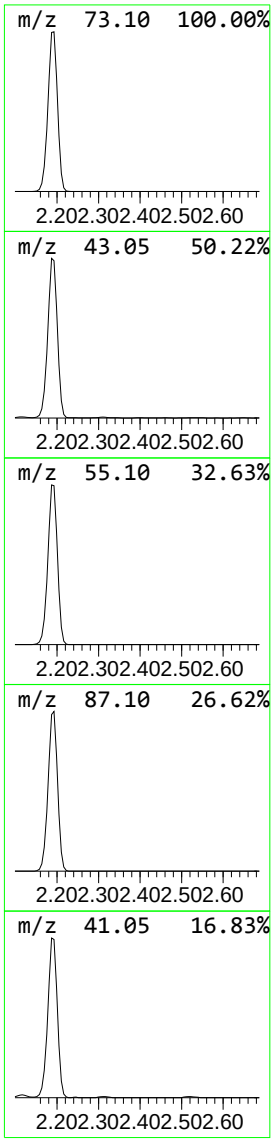
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.187	62.82 ng	1308150	1,4-Dichlorobenzene-d4	6.875

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	40
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
4	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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Acq On : 18 Sep 2024 20:44
Operator : RC/JU
Sample : P4023-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONCRETE-TP-9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

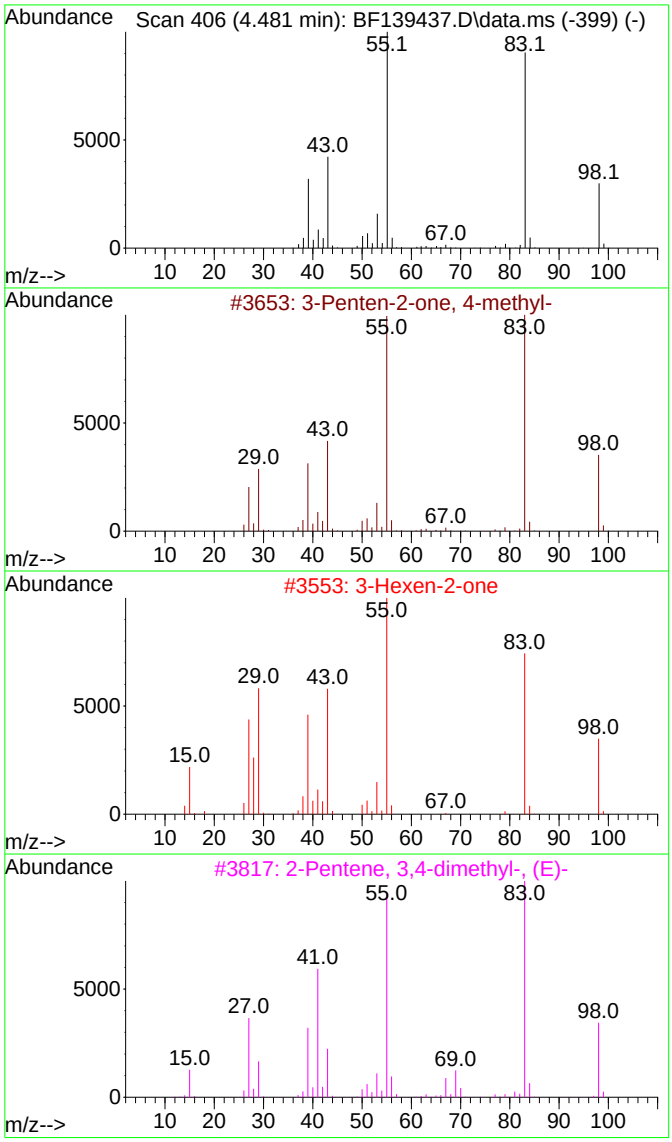
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

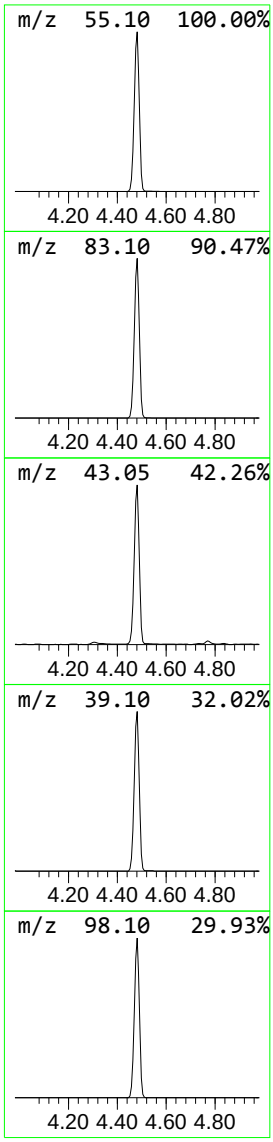
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.481	41.42 ng	862594	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
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





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091824\
Data File : BF139437.D
Acq On : 18 Sep 2024 20:44
Operator : RC/JU
Sample : P4023-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONCRETE-TP-9

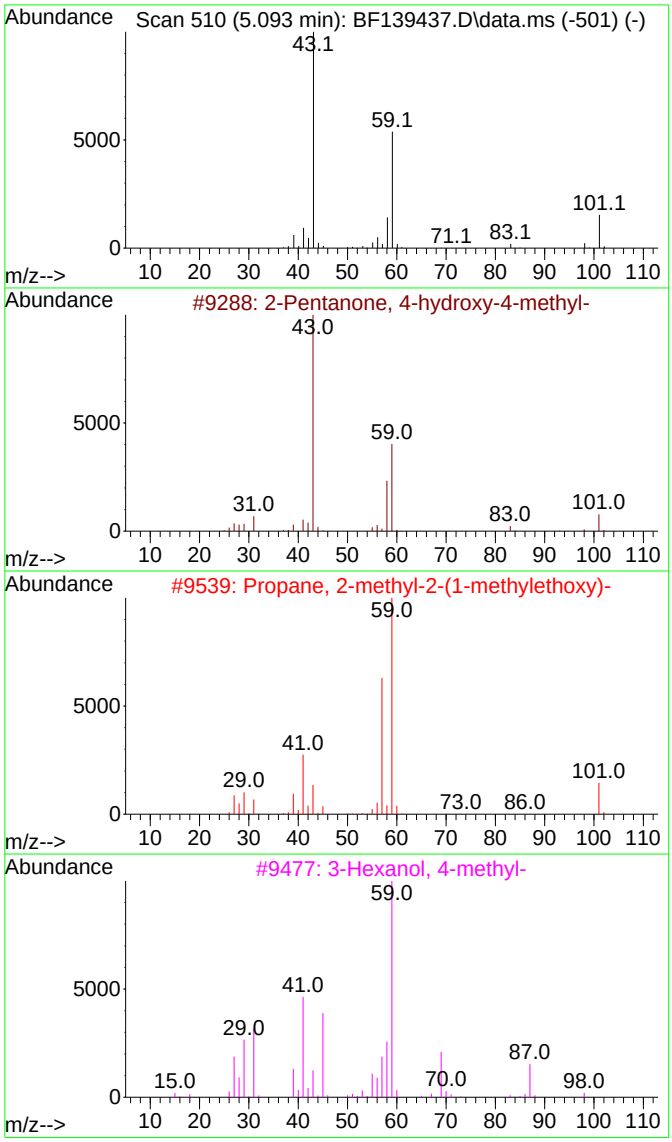
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

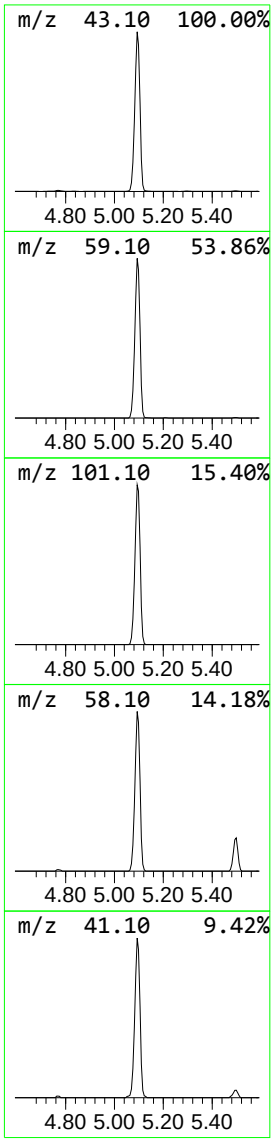
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	34.11 ng	710429	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28





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Acq On : 18 Sep 2024 20:44
Operator : RC/JU
Sample : P4023-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONCRETE-TP-9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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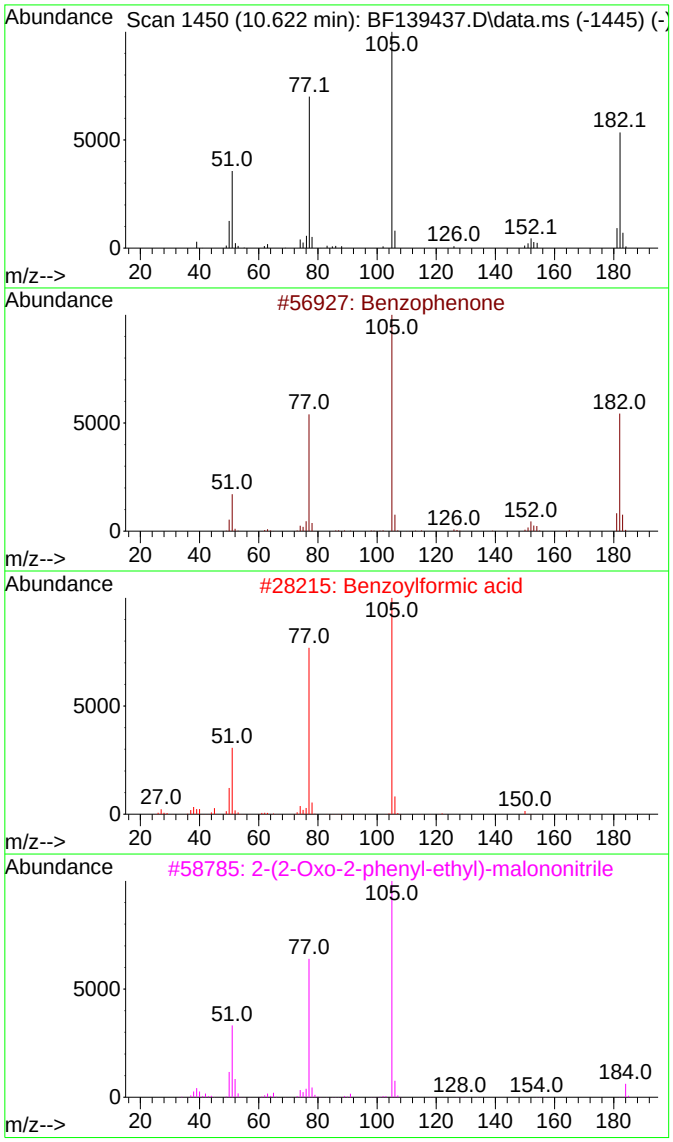
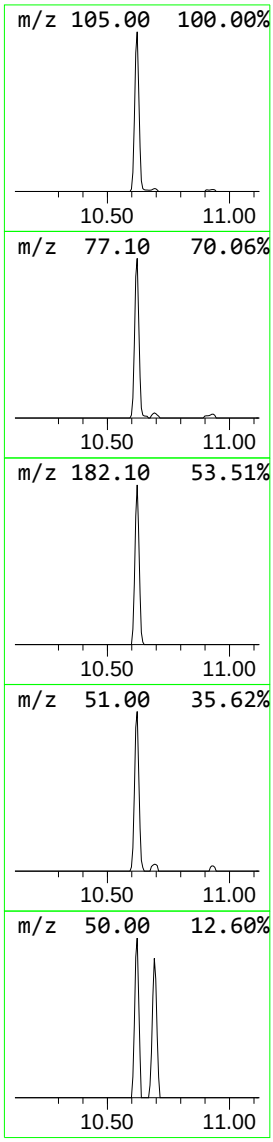
Peak Number 4 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.622	3.31 ng	80198	Acenaphthene-d10	9.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzoylformic acid	150	C8H6O3	000611-73-4	60
3	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	49
4	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
5	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091824\
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Operator : RC/JU
Sample : P4023-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONCRETE-TP-9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

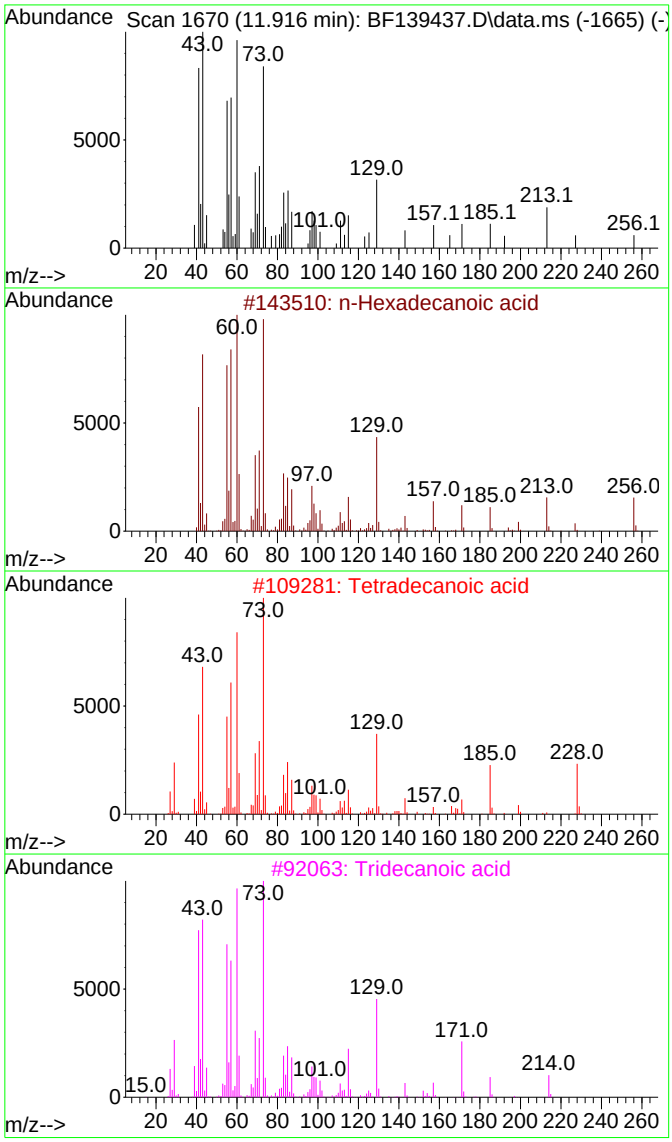
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

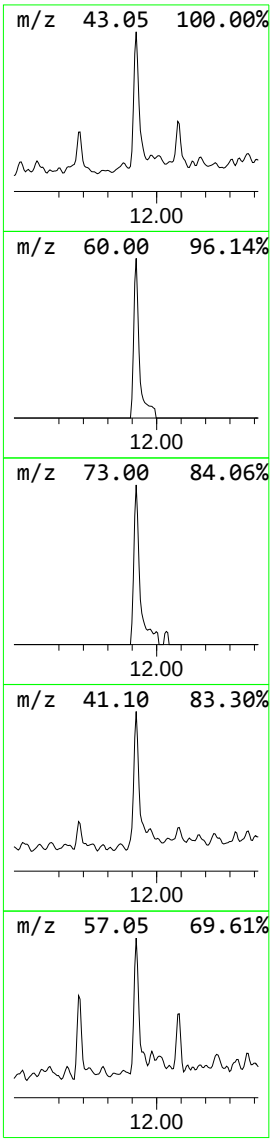
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	2.54 ng	51492	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3	Tridecanoic acid	214	C13H26O2	000638-53-9	80
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONCRETE-TP-9

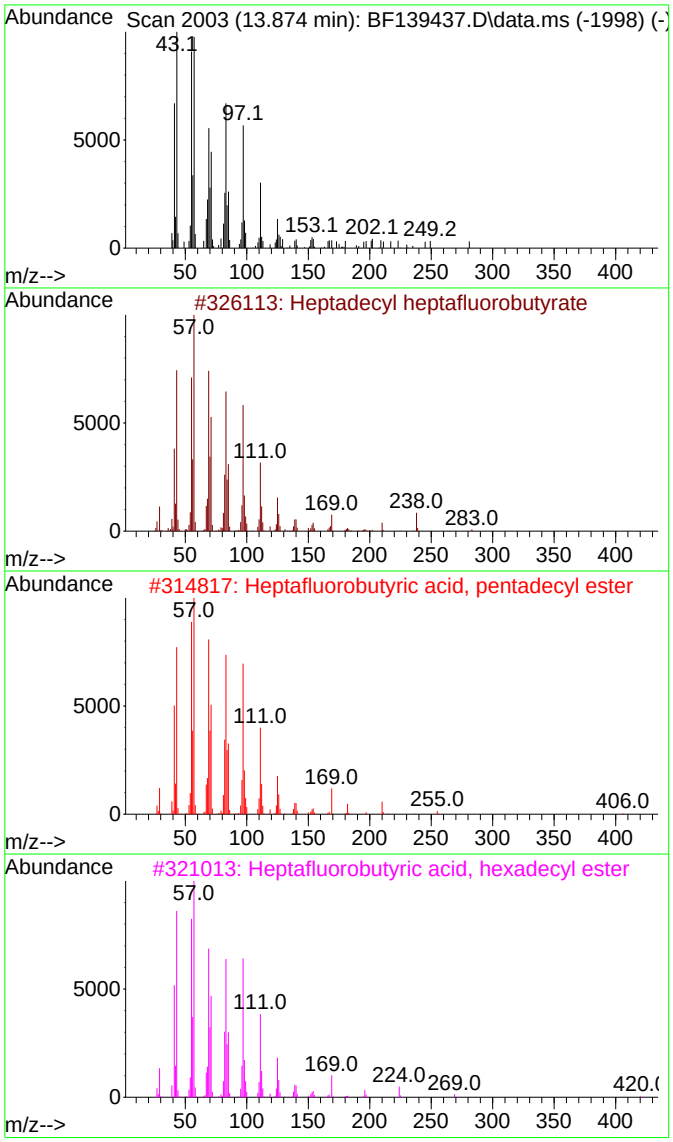
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

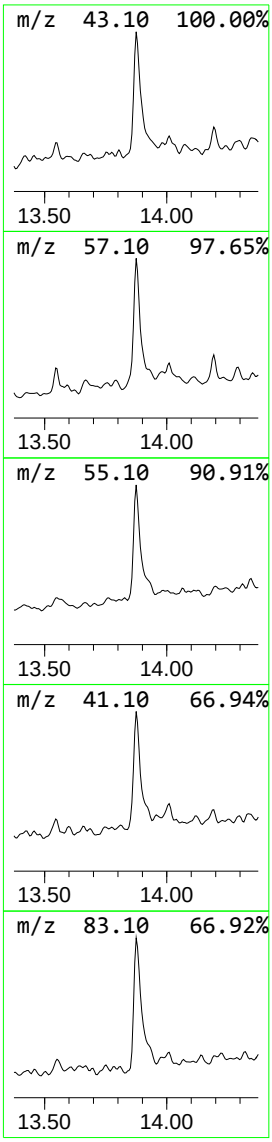
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	6.63 ng	115026	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91





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BNA_F
ClientSampleId :
CONCRETE-TP-9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.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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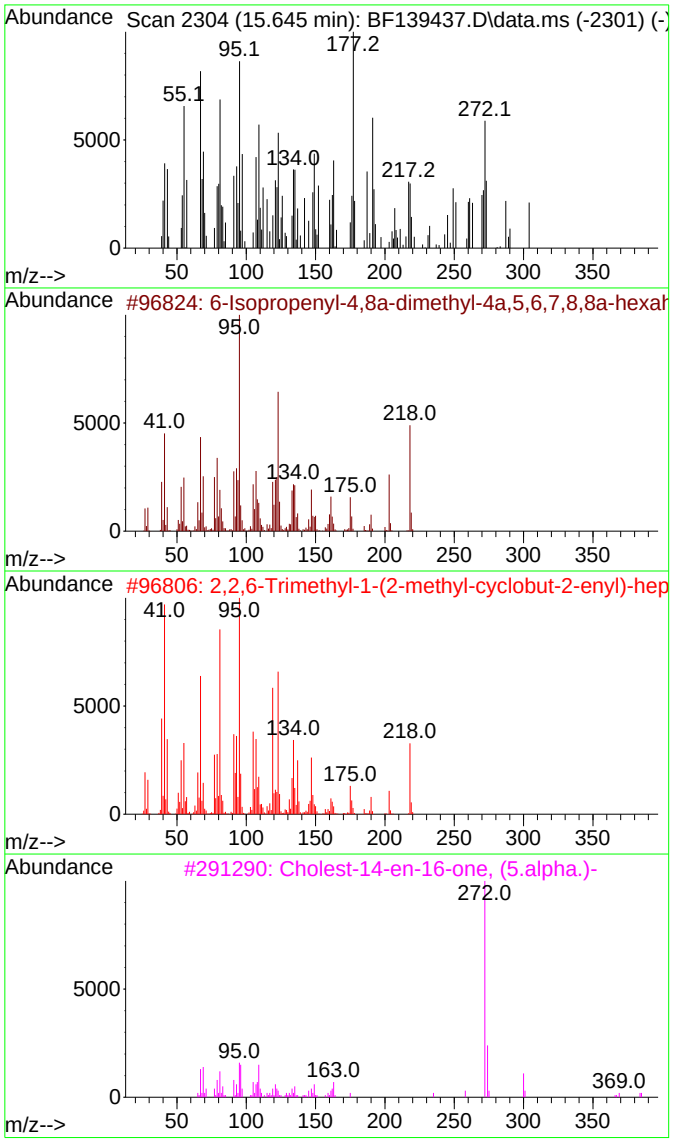
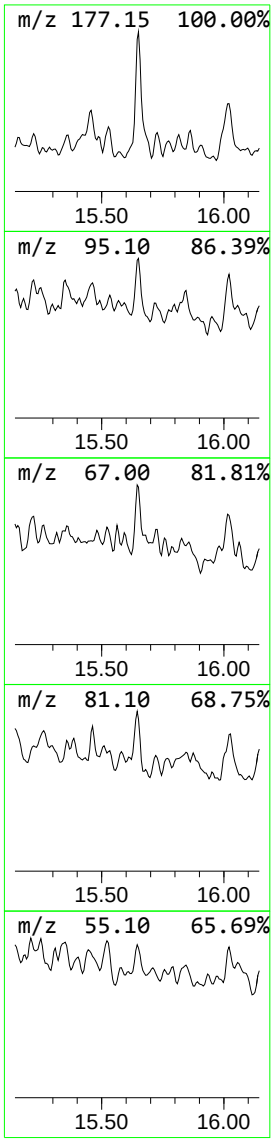
Peak Number 7 unknown15.645 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.645	2.27 ng	30987	Perylene-d12	15.498

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Isopropenyl-4,8a-dimethyl-4a,5...	218	C15H22O	086917-79-5	25
2	2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	25
3	Cholest-14-en-16-one, (5.alpha.)-	384	C27H44O	054725-43-8	22
4	1-(4-Fluorophenyl)-1H-pyrazol-5-...	177	C9H8FN3	727967-95-5	18
5	Quinoline, 2-chloro-6-methyl-	177	C10H8ClN	004295-11-8	11





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091824\
Data File : BF139437.D
Acq On : 18 Sep 2024 20:44
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.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...	2.187	62.8	ng	1308150	1	6.875	416502	20.0
3-Penten-2-one,...	4.481	41.4	ng	862594	1	6.875	416502	20.0
2-Pentanone, 4-...	5.093	34.1	ng	710429	1	6.875	416502	20.0
Benzophenone	10.622	3.3	ng	80198	3	9.910	484240	20.0
n-Hexadecanoic ...	11.916	2.5	ng	51492	4	11.392	405127	20.0
Heptadecyl hept...	13.874	6.6	ng	115026	5	14.027	347107	20.0
unknown15.645	15.645	2.3	ng	30987	6	15.498	273331	20.0