LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102924\
Data File : BF140128.D
Acq On : 29 Oct 2024 22:31
Operator : RC/JU
Sample : P4598-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F12

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-BF101824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140128.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	10	18	27	rVB	970005	1563427	60.67%	8.210%
2	2.299	30	35	50	rVB	15573	29013	1.13%	0.152%
3	4.505	405	410	417	rBV	125523	179526	6.97%	0.943%
4	5.116	506	514	522	rVB	73460	112723	4.37%	0.592%
5	5.510	574	581	586	rBV	1582041	2117573	82.17%	11.120%
6	6.510	744	751	756	rBV	1529107	2140450	83.06%	11.240%
7	6.887	810	815	820	rBV	622164	770178	29.89%	4.044%
8	7.445	904	910	915	rBV	1121331	1454922	56.46%	7.640%
9	7.698	949	953	962	rVB	37626	46072	1.79%	0.242%
10	8.169	1027	1033	1038	rBV	817171	1011104	39.24%	5.310%
11	9.245	1210	1216	1236	rBV	1929360	2576924	100.00%	13.532%
12	9.922	1326	1331	1346	rBB	822314	1047599	40.65%	5.501%
13	10.634	1447	1452	1460	rBV	386225	491528	19.07%	2.581%
14	10.710	1460	1465	1481	rVB	885934	1130916	43.89%	5.939%
15	10.945	1500	1505	1516	rVB	59289	74290	2.88%	0.390%
16	11.410	1579	1584	1591	rBV	675432	838244	32.53%	4.402%
17	11.933	1667	1673	1688	rBV2	104094	185769	7.21%	0.976%
18	12.716	1802	1806	1817	rBV3	14532	29353	1.14%	0.154%
19	12.998	1848	1854	1868	rBV	1312034	1726577	67.00%	9.067%
20	13.898	2001	2007	2025	rBV2	39870	114207	4.43%	0.600%
21	14.051	2028	2033	2043	rVV	522318	686502	26.64%	3.605%
22	14.821	2159	2164	2175	rBV3	41649	90160	3.50%	0.473%
23	15.539	2280	2286	2297	rBV	378423	626146	24.30%	3.288%

Sum of corrected areas: 19043203

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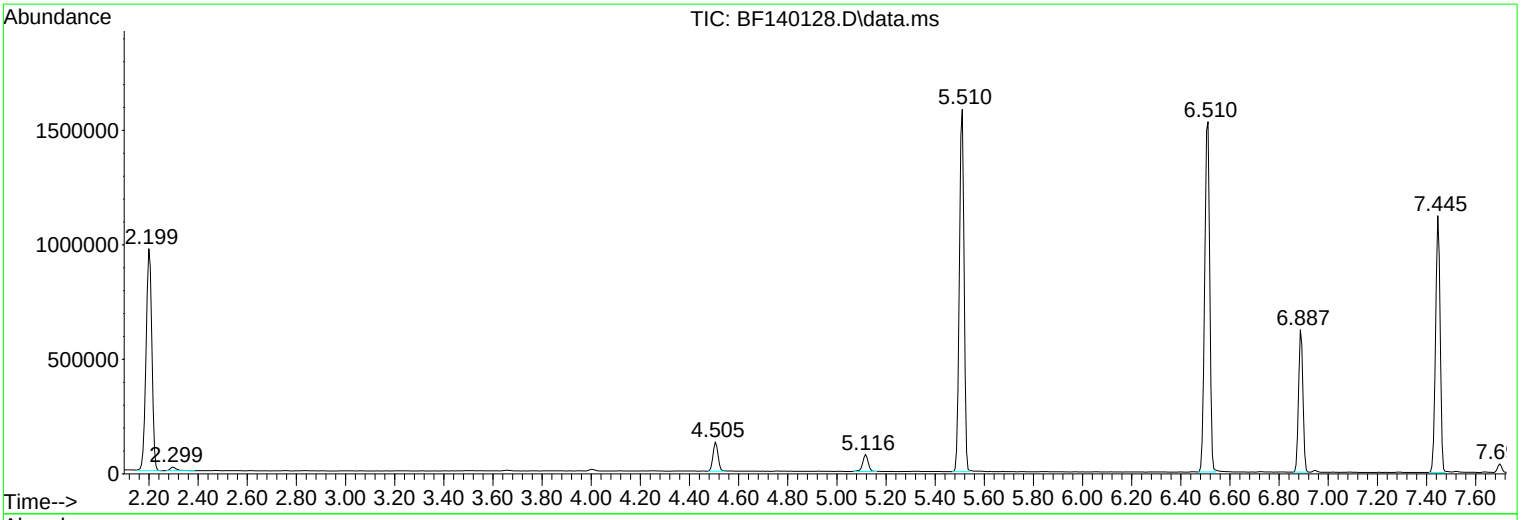
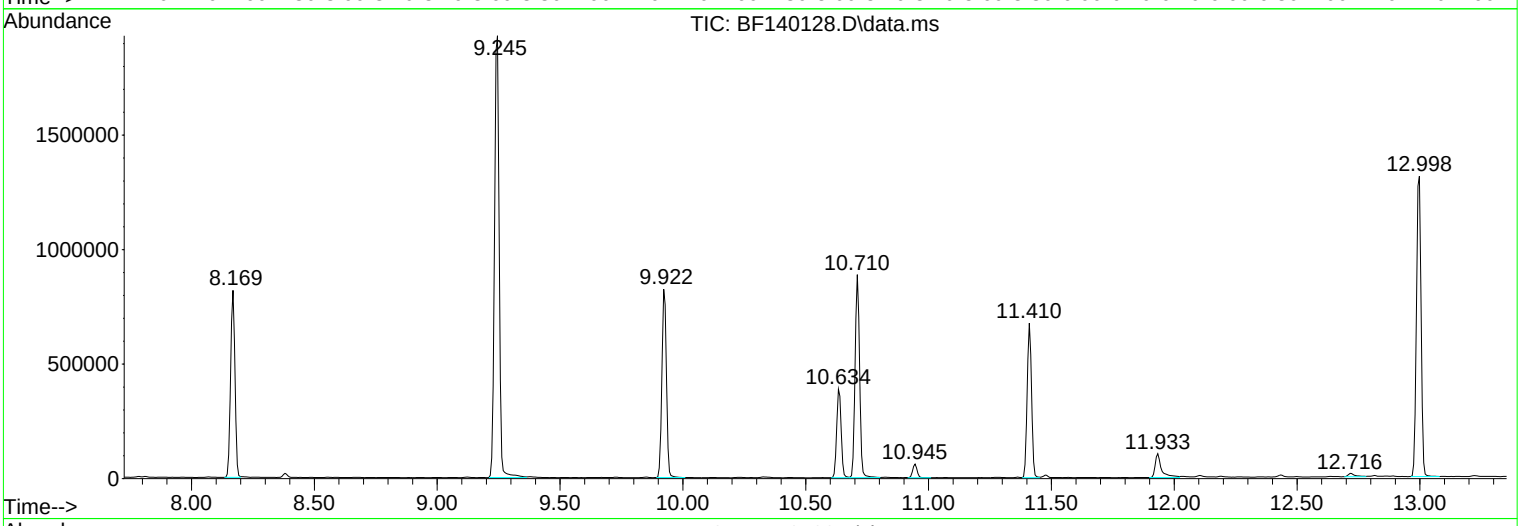
Misc :
ALS Vial : 17 Sample Multiplier: 1

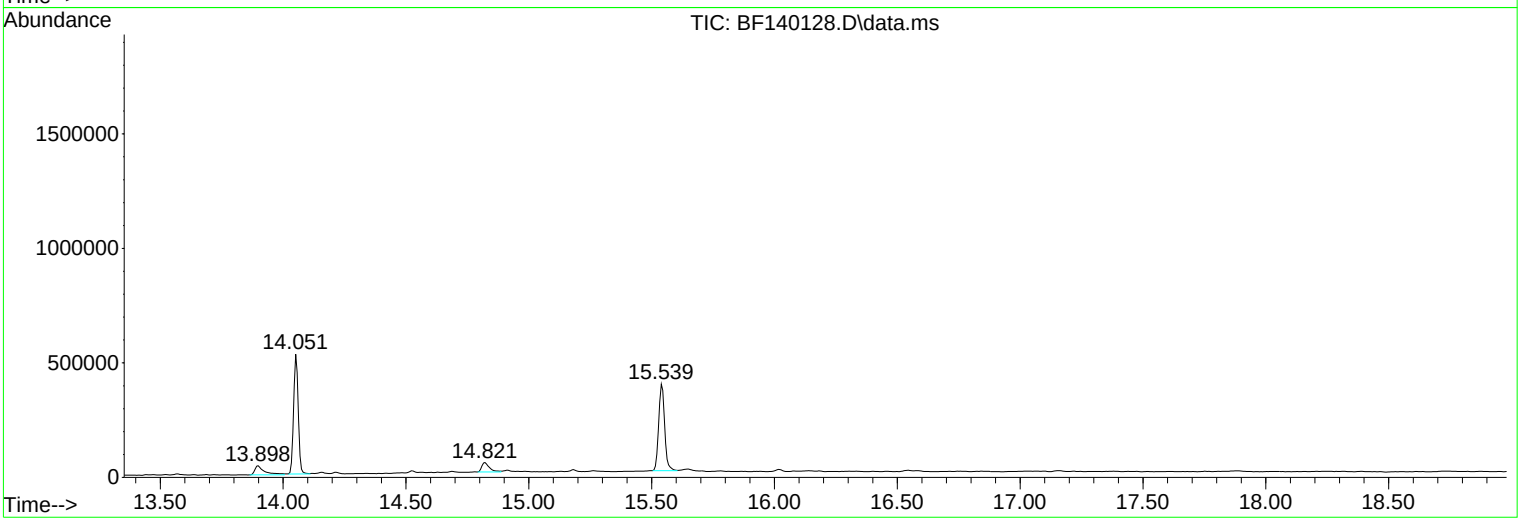
Instrument :
BNA_F
ClientSampleId :
BP-F12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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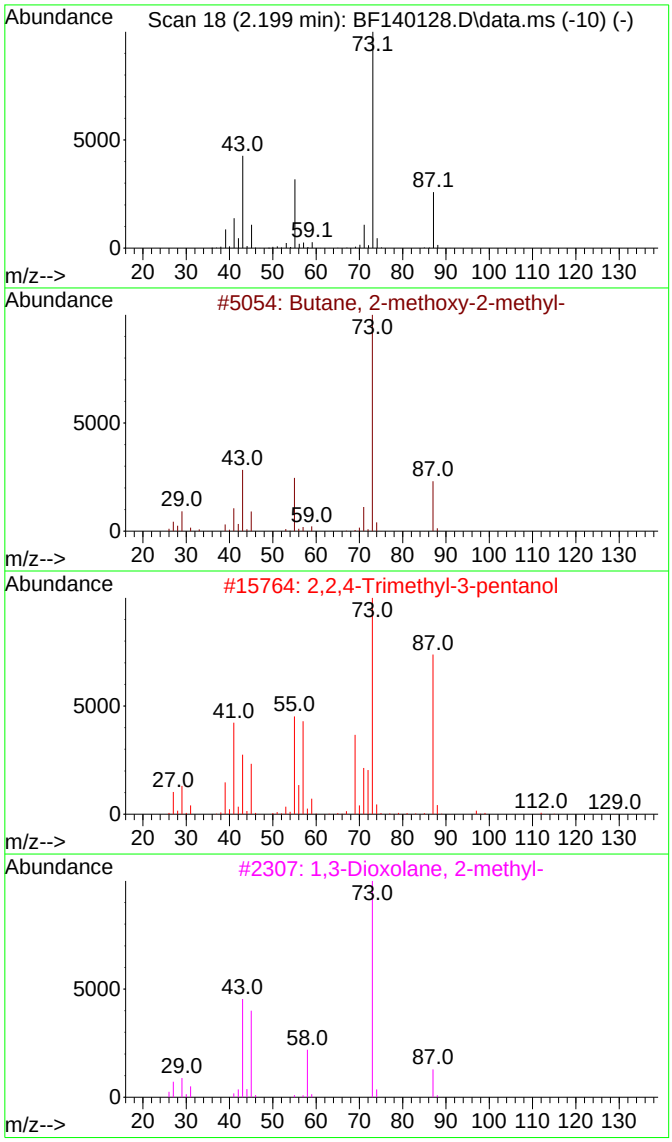
TIC Integration Parameters: LSCINT.P

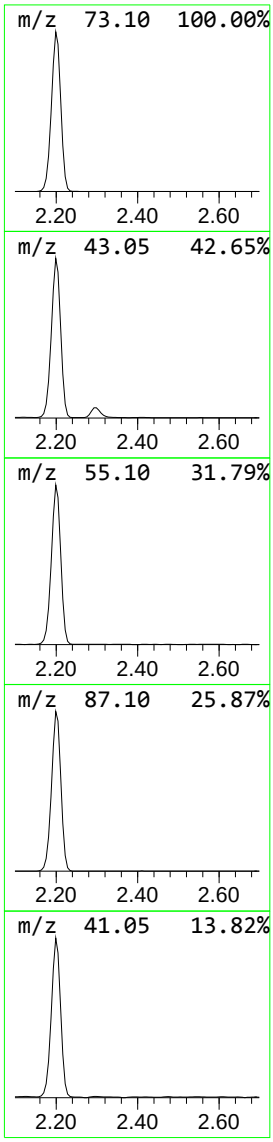
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	40.60 ng	1563430	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	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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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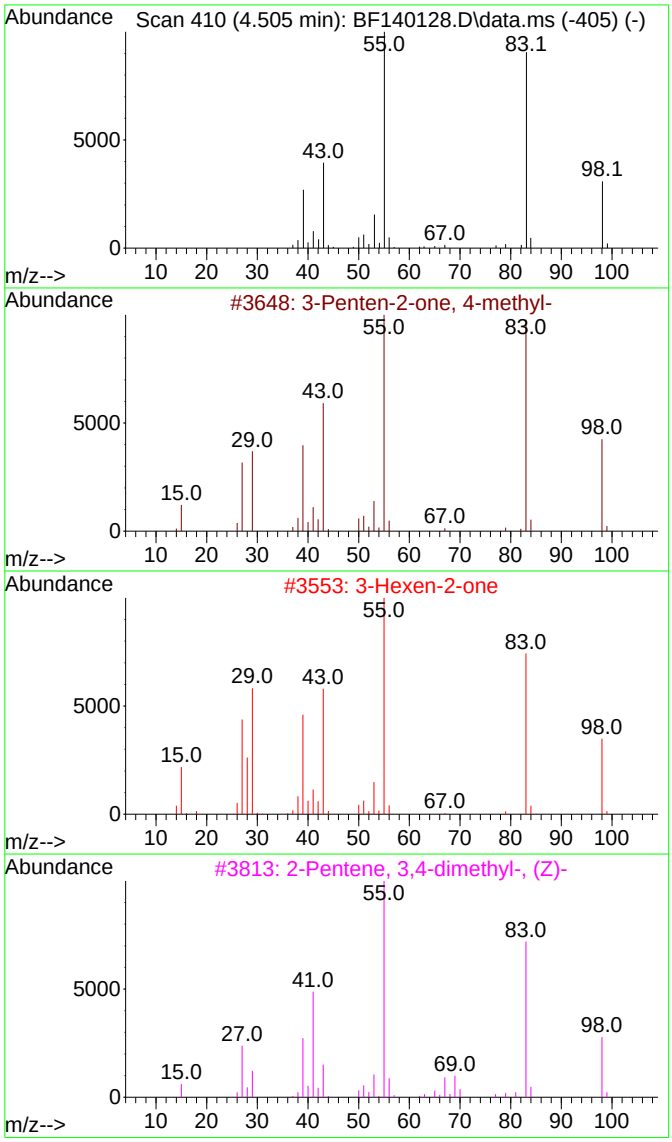
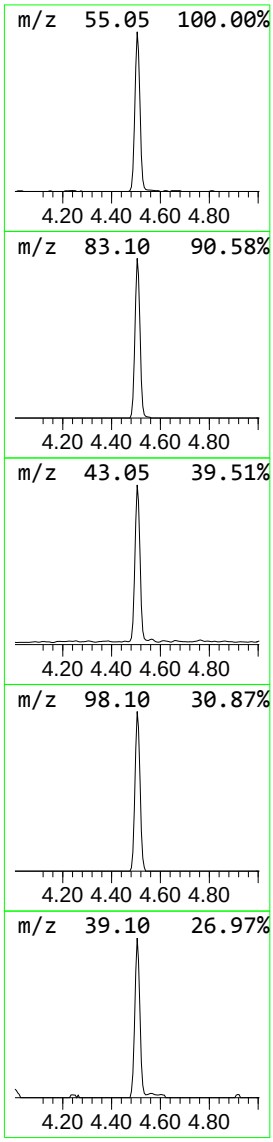
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.505	4.66 ng	179526	1,4-Dichlorobenzene-d4	6.887

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-, (Z)-	98	C7H14	004914-91-4	86
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78





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Operator : RC/JU
Sample : P4598-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F12

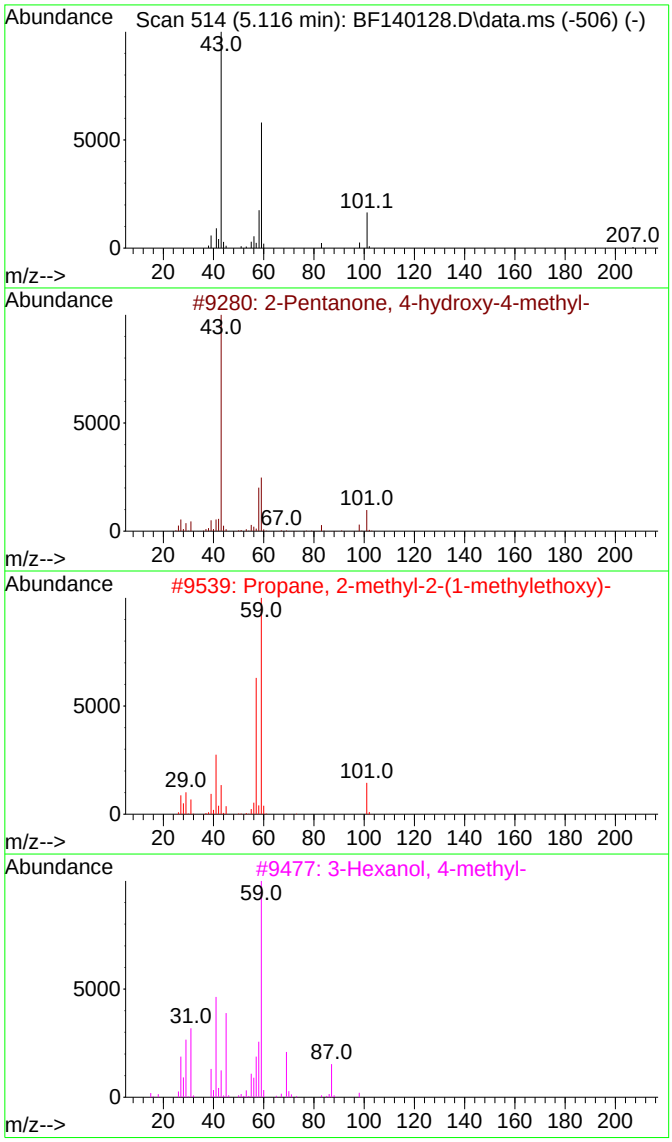
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

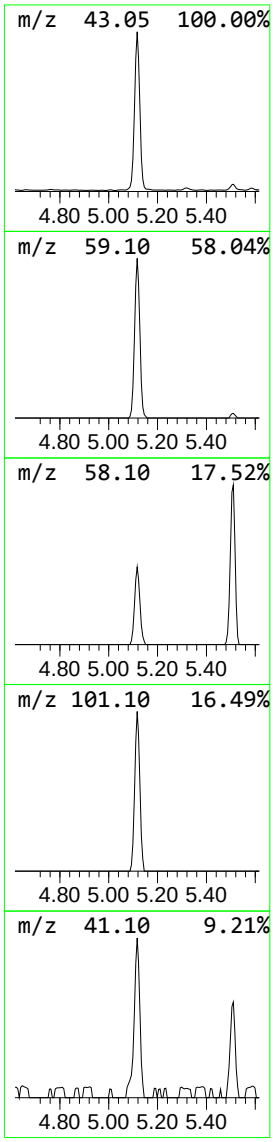
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	2.93 ng	112723	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
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	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





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Sample : P4598-01
Misc :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
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TIC Library : C:\Database\NIST20.L
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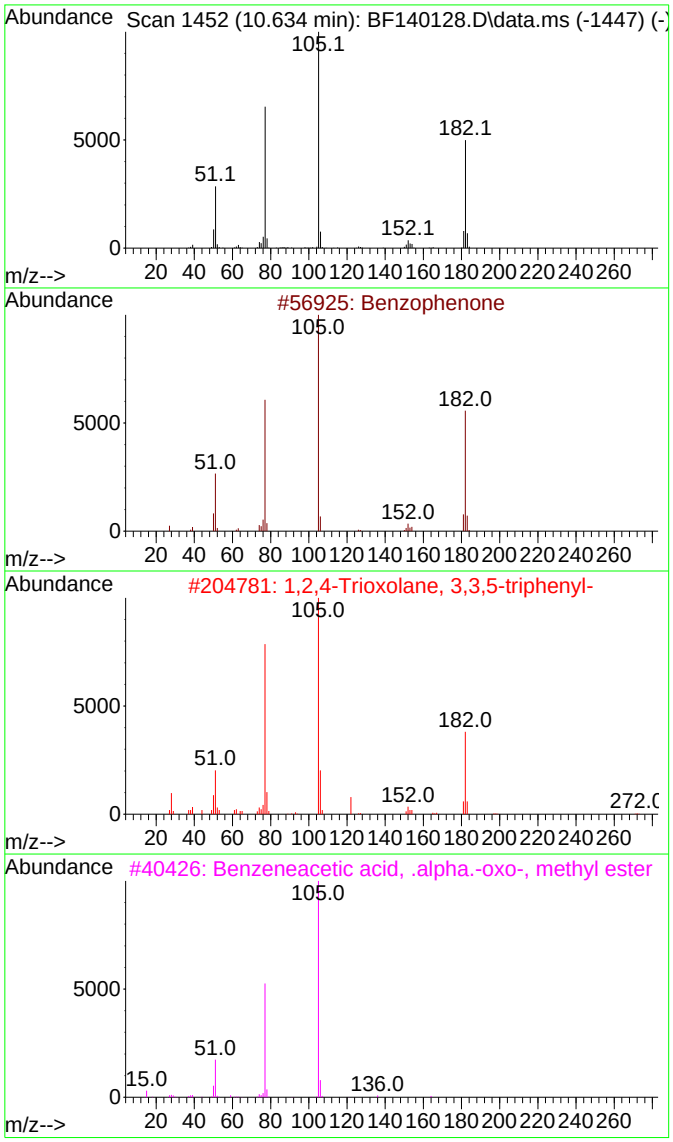
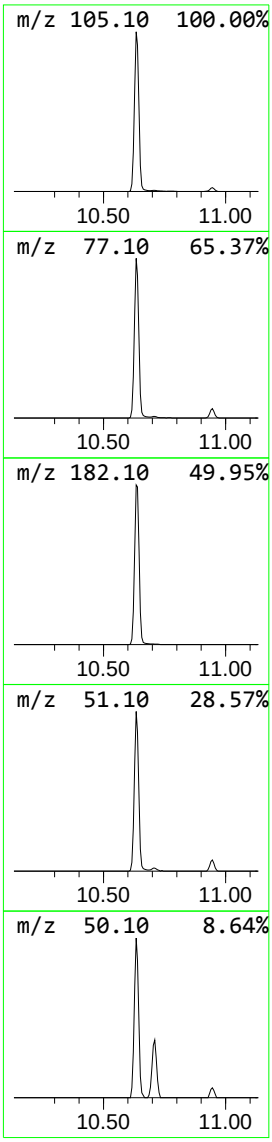
Peak Number 4 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.634	9.38 ng	491528	Acenaphthene-d10	9.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	72
3	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	49
4	2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47
5	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	47





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BP-F12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
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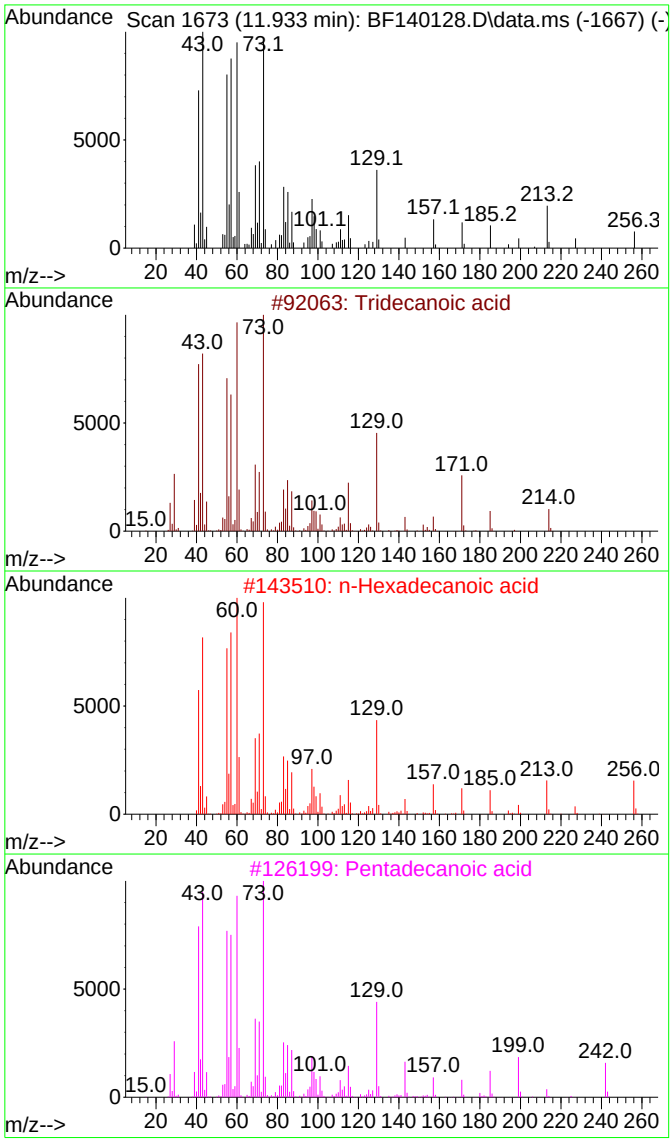
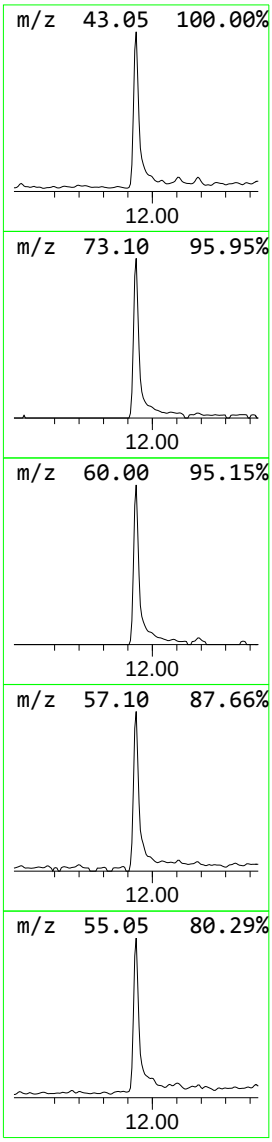
****

Peak Number 5 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	4.43 ng	185769	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	94
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





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BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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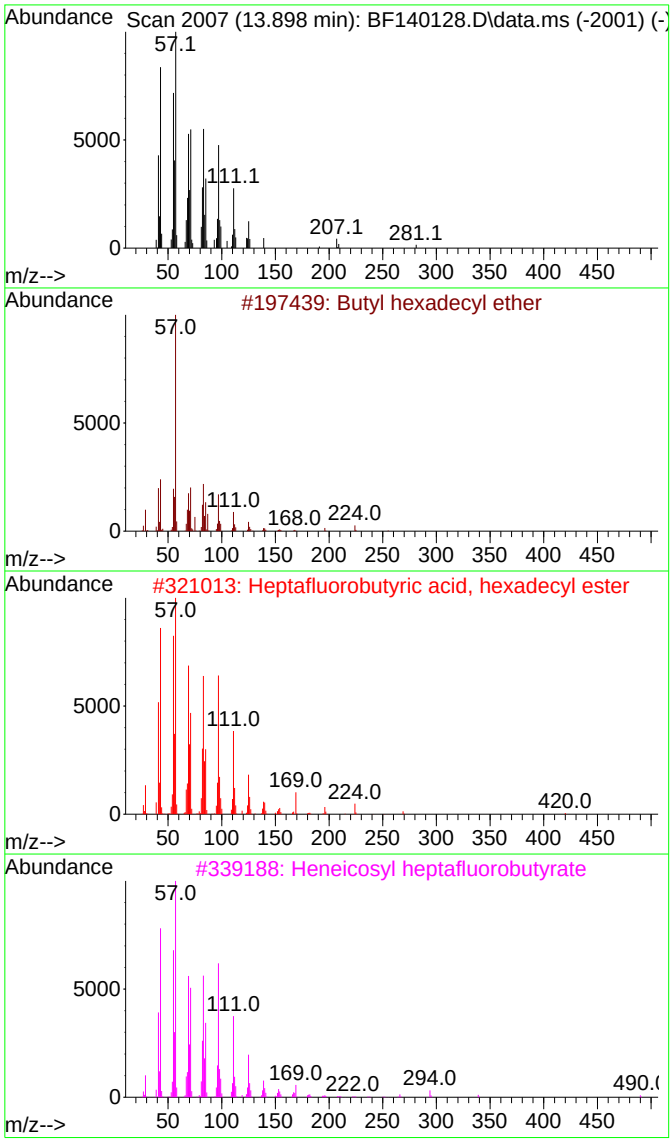
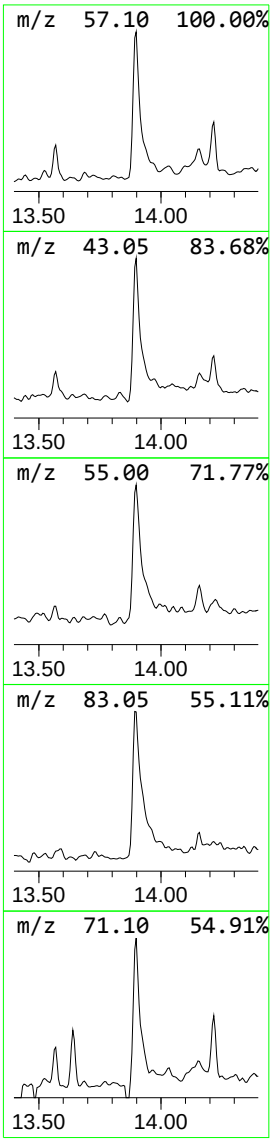
Peak Number 6 Butyl hexadecyl ether Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	3.33 ng	114207	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl hexadecyl ether	298	C20H42O	1010406-40-5	91
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
3	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
4	17-Pentatriacontene	491	C35H70	006971-40-0	91
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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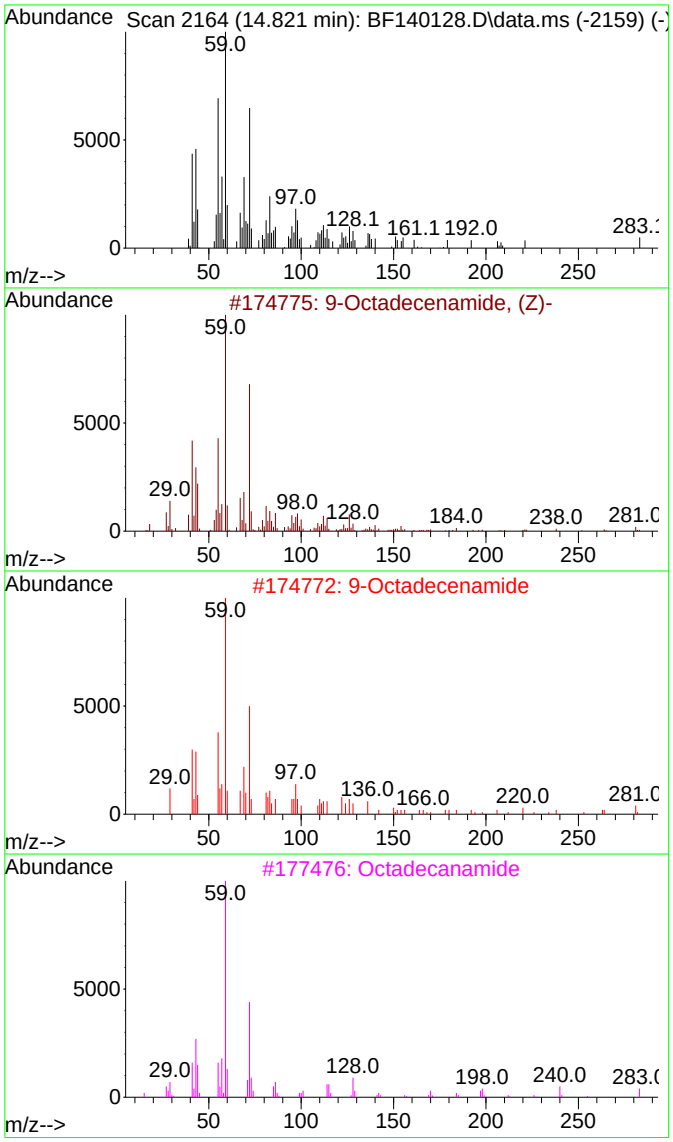
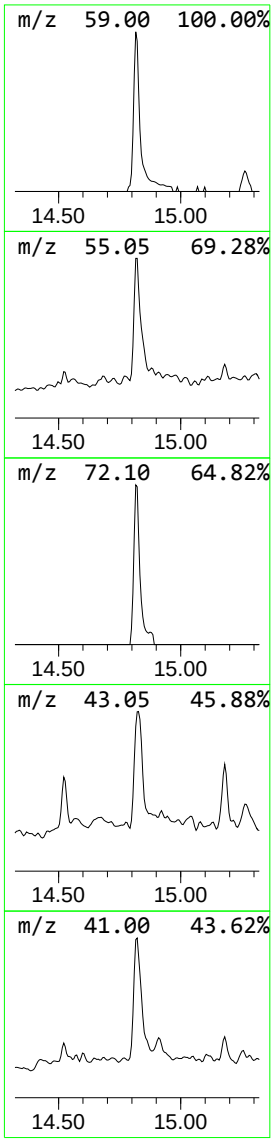
Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.822	2.88 ng	90160	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
2	9-Octadecenamide	281	C18H35NO	003322-62-1	80
3	Octadecanamide	283	C18H37NO	000124-26-5	58
4	d-Glucosamine	179	C6H13NO5	000090-77-7	53
5	Tetradecanamide	227	C14H29NO	000638-58-4	53





Tentatively Identified Compound (LSC) summary

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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...	2.199	40.6	ng	1563430	1	6.887	770178	20.0
3-Penten-2-one,...	4.505	4.7	ng	179526	1	6.887	770178	20.0
2-Pentanone, 4-...	5.116	2.9	ng	112723	1	6.887	770178	20.0
Benzophenone	10.634	9.4	ng	491528	3	9.922	1047600	20.0
Tridecanoic acid	11.933	4.4	ng	185769	4	11.410	838244	20.0
Butyl hexadecyl...	13.898	3.3	ng	114207	5	14.051	686502	20.0
9-Octadecenamid...	14.822	2.9	ng	90160	6	15.539	626146	20.0