LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092624\
Data File : BF139566.D
Acq On : 27 Sep 2024 00:45
Operator : RC/JU
Sample : P4198-26
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP5-WC-1

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: BF139566.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	5	13	27	rVB	1847883	2898965	100.00%	20.220%
2	3.381	213	219	239	rBV	37769	94281	3.25%	0.658%
3	5.093	500	510	517	rBV	80989	127287	4.39%	0.888%
4	5.498	573	579	584	rBV	1232389	1646906	56.81%	11.487%
5	6.504	744	750	755	rBV	1320560	1743454	60.14%	12.161%
6	6.875	808	813	818	rBV	245912	289944	10.00%	2.022%
7	7.434	903	908	914	rBV	804452	1067163	36.81%	7.443%
8	8.157	1026	1031	1047	rVB	305142	373265	12.88%	2.604%
9	8.469	1079	1084	1097	rBV	52766	75843	2.62%	0.529%
10	9.228	1208	1213	1223	rBV	1316641	1716922	59.23%	11.975%
11	9.910	1324	1329	1339	rBV	329101	405504	13.99%	2.828%
12	10.004	1339	1345	1352	rVB	38995	58016	2.00%	0.405%
13	10.698	1458	1463	1479	rBV	843769	1089988	37.60%	7.603%
14	11.398	1576	1582	1589	rBV	325153	428740	14.79%	2.990%
15	11.916	1664	1670	1679	rBV2	32570	59357	2.05%	0.414%
16	12.980	1845	1851	1856	rBV	1342266	1673222	57.72%	11.671%
17	13.886	1999	2005	2019	rBV6	13311	42775	1.48%	0.298%
18	14.033	2025	2030	2038	rVB	211956	275616	9.51%	1.922%
19	15.504	2274	2280	2294	rVB	169737	269751	9.31%	1.882%

Sum of corrected areas: 14336999

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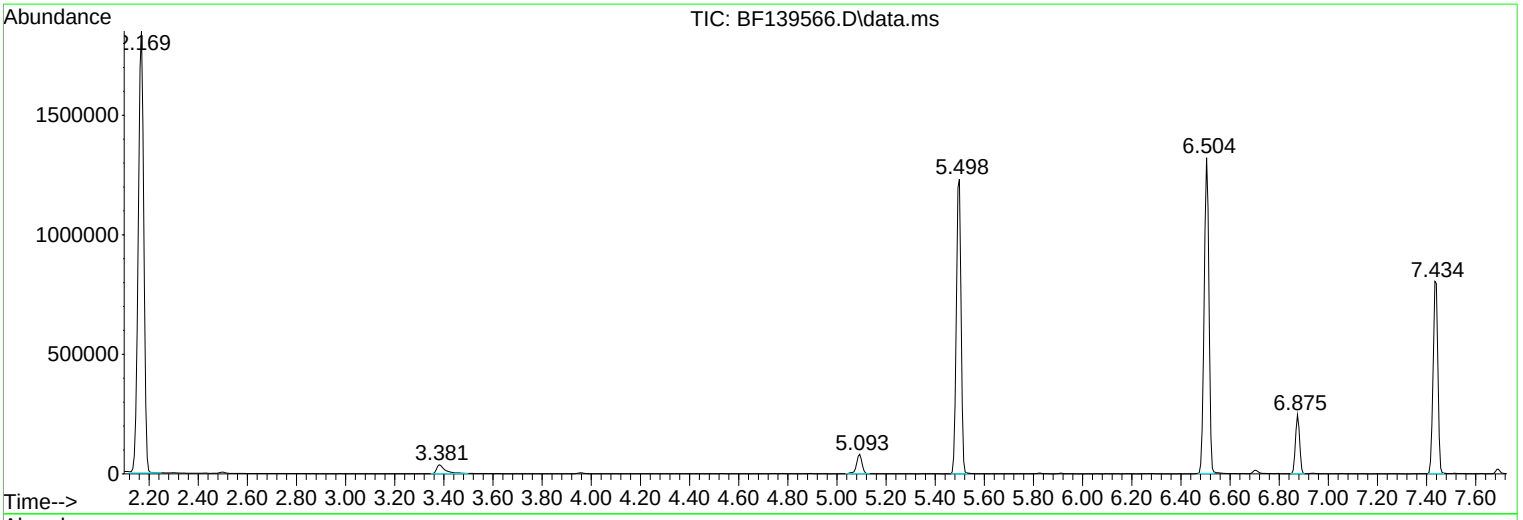
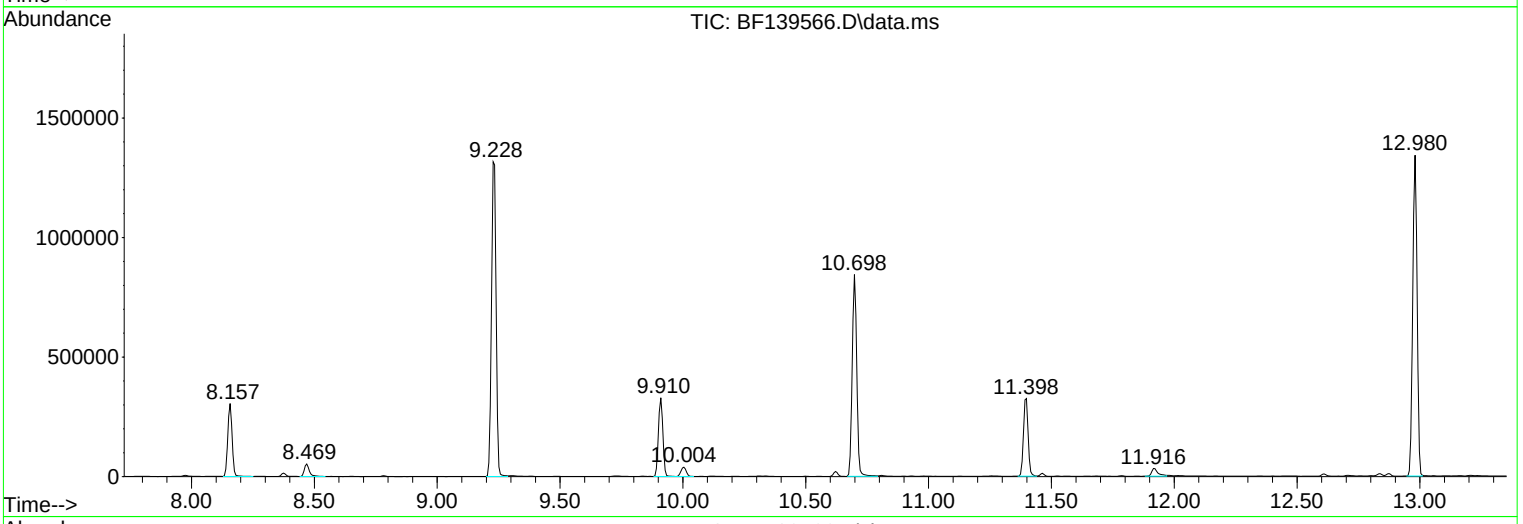
Misc :
ALS Vial : 21 Sample Multiplier: 1

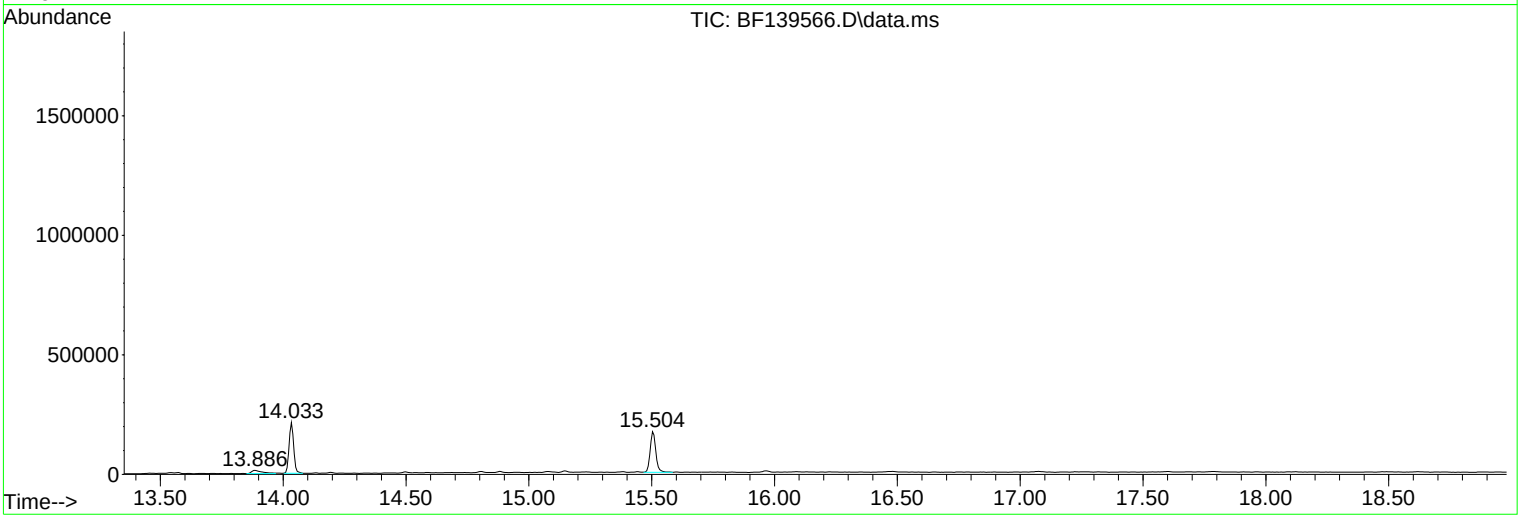
Instrument :
BNA_F
ClientSampleId :
TP5-WC-1

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 : BF139566.D
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

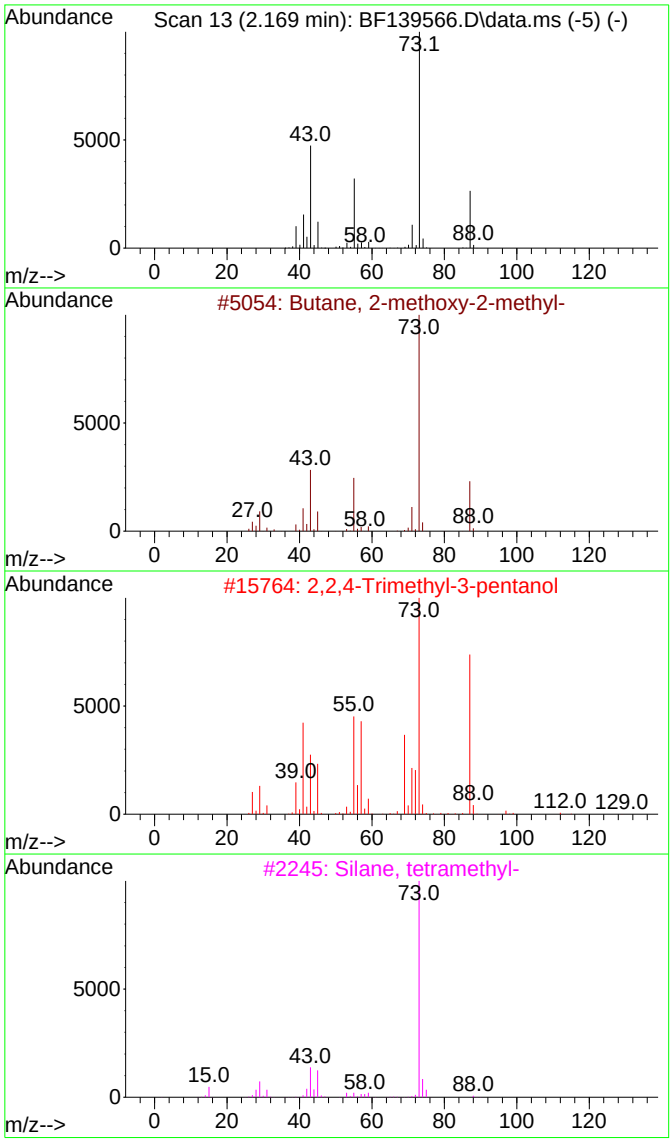
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

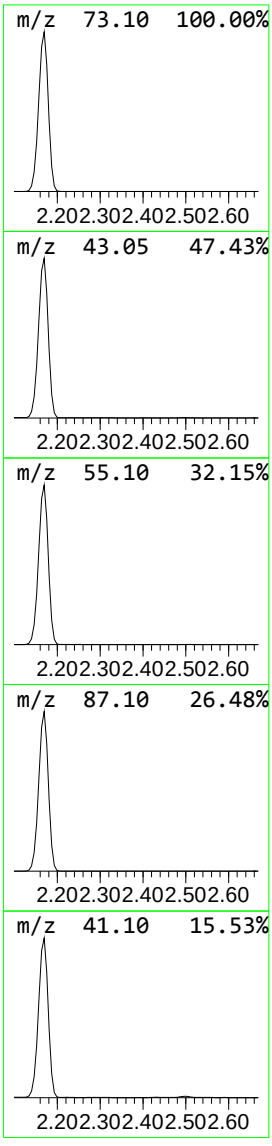
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	199.97 ng	2898970	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	38
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





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Operator : RC/JU
Sample : P4198-26
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP5-WC-1

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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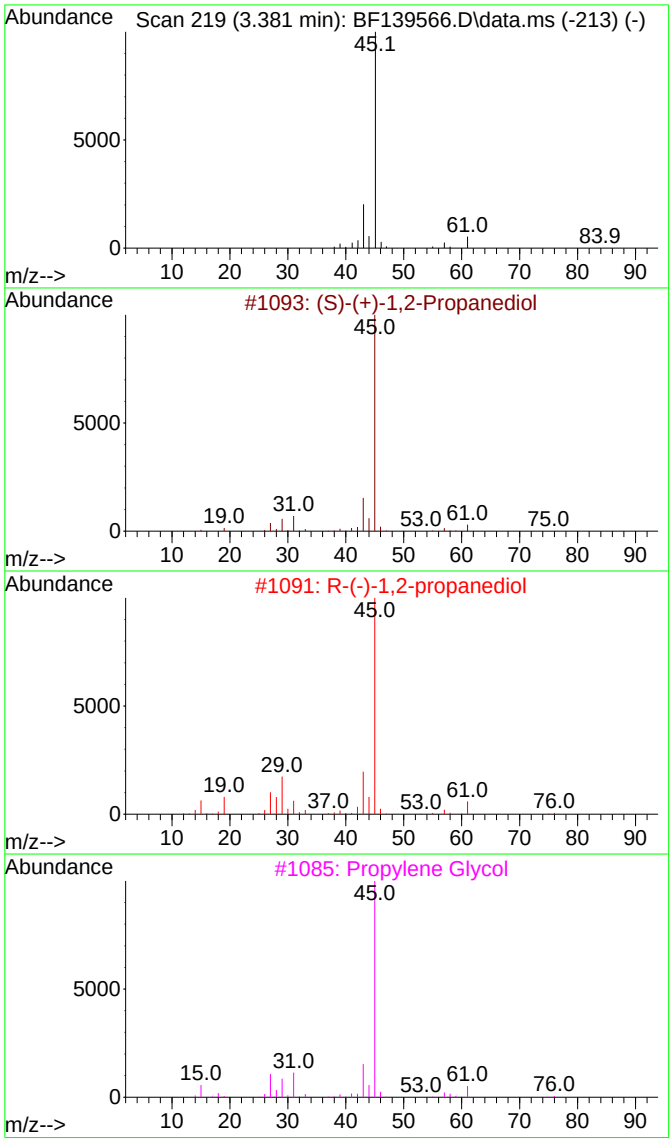
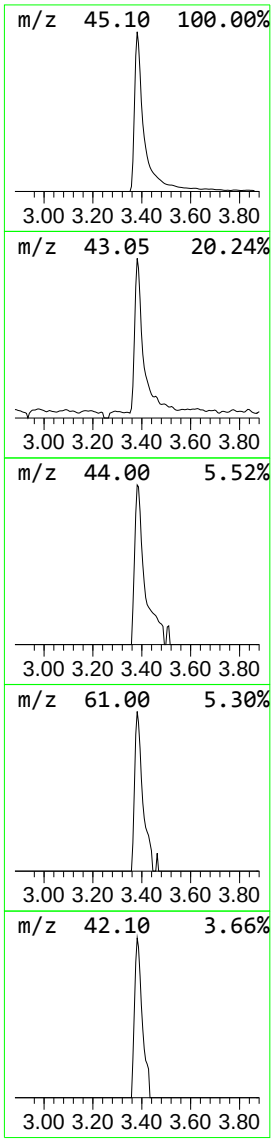
Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.381	6.50 ng	94281	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
3	Propylene Glycol	76	C3H8O2	000057-55-6	9
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9





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Data File : BF139566.D
Acq On : 27 Sep 2024 00:45
Operator : RC/JU
Sample : P4198-26
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP5-WC-1

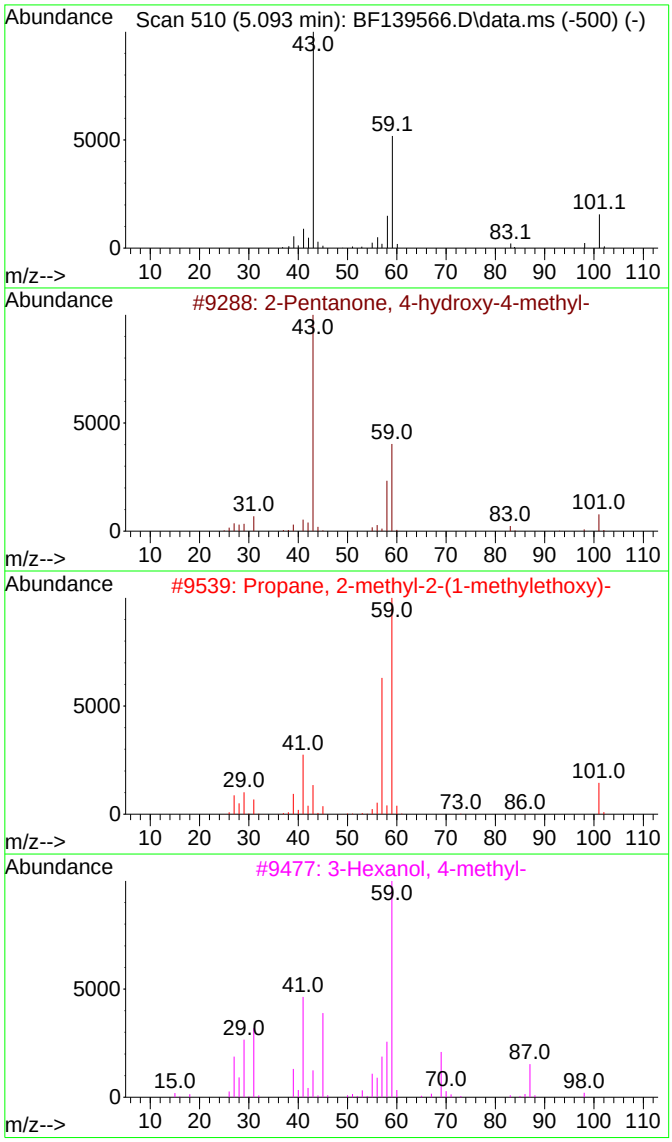
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

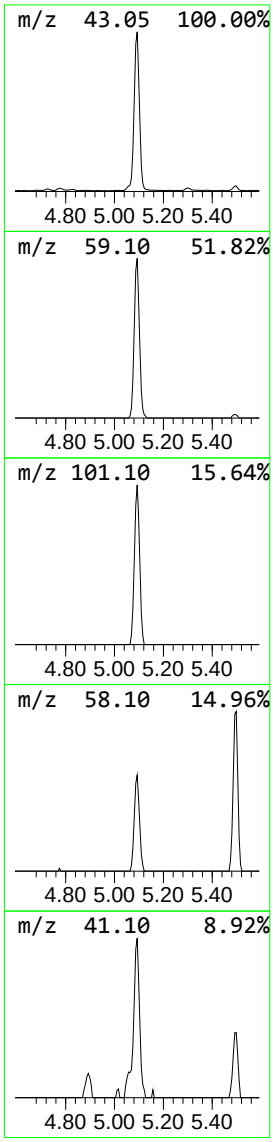
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	8.78 ng	127287	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	56
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	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28





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Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP5-WC-1

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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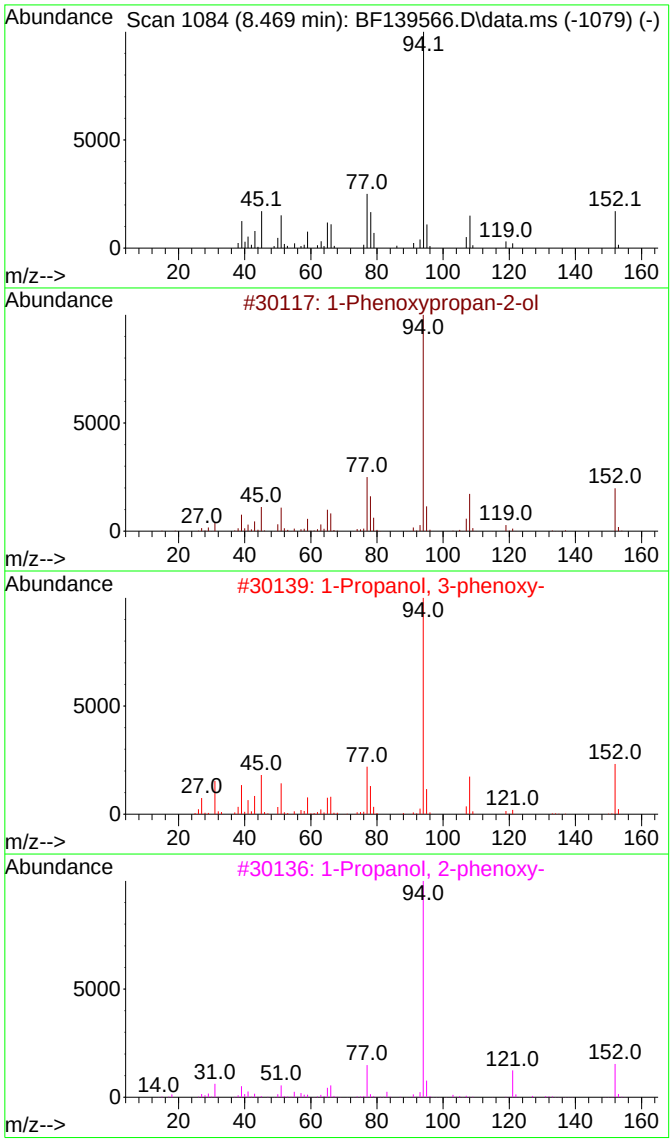
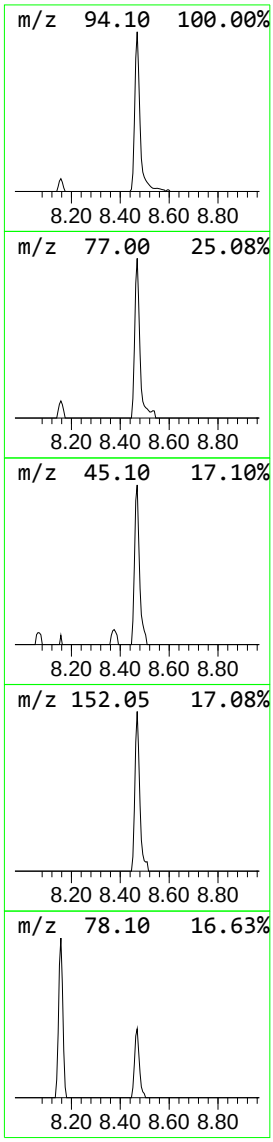
Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.469	4.06 ng	75843	Naphthalene-d8	8.157

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	97
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	91
3	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
4	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
5	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59





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Instrument :
BNA_F
ClientSampleId :
TP5-WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
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TIC Library : C:\Database\NIST20.L
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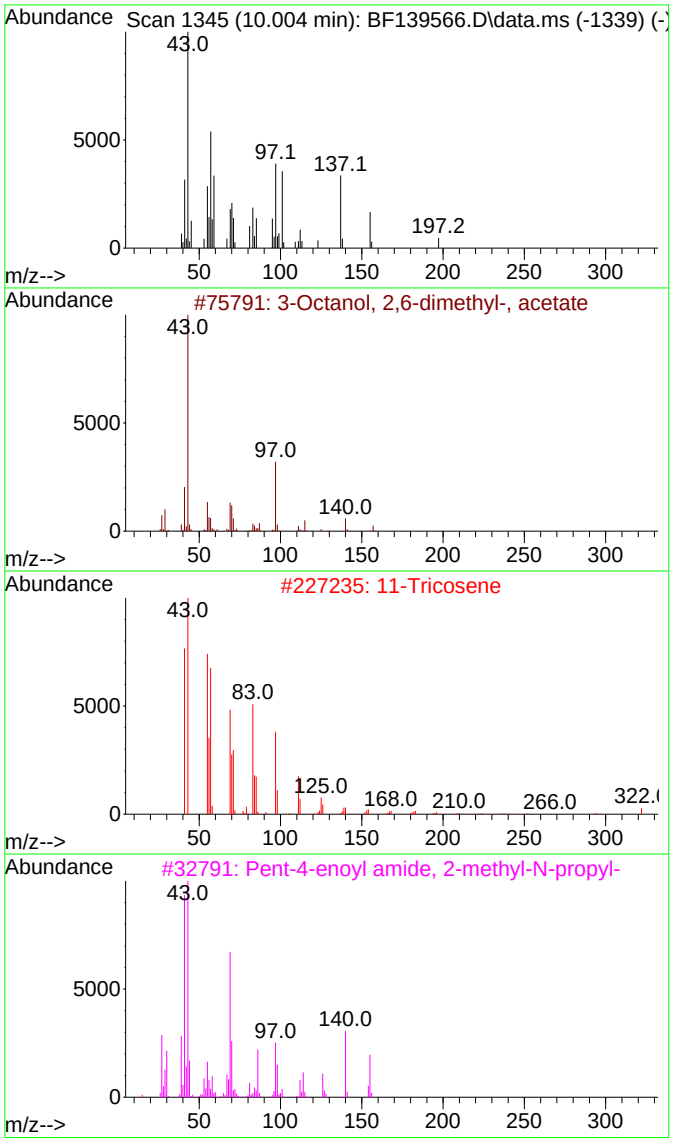
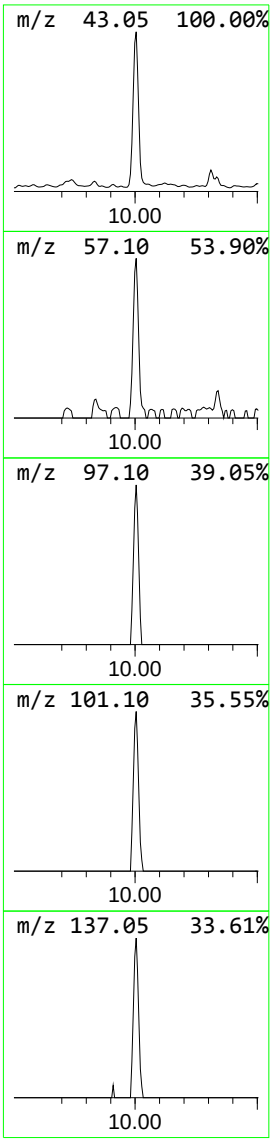
****

Peak Number 5 unknown10.004 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.004	2.86 ng	58016	Acenaphthene-d10	9.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octanol, 2,6-dimethyl-, acetate	200	C12H24O2	123232-57-5	27
2	11-Tricosene	322	C23H46	052078-56-5	25
3	Pent-4-enoyl amide, 2-methyl-N-p...	155	C9H17NO	1000420-35-2	14
4	4-Dodecanol, acetate	228	C14H28O2	060826-25-7	12
5	Heptacosyl acetate	438	C29H58O2	1000351-78-2	10





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ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP5-WC-1

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

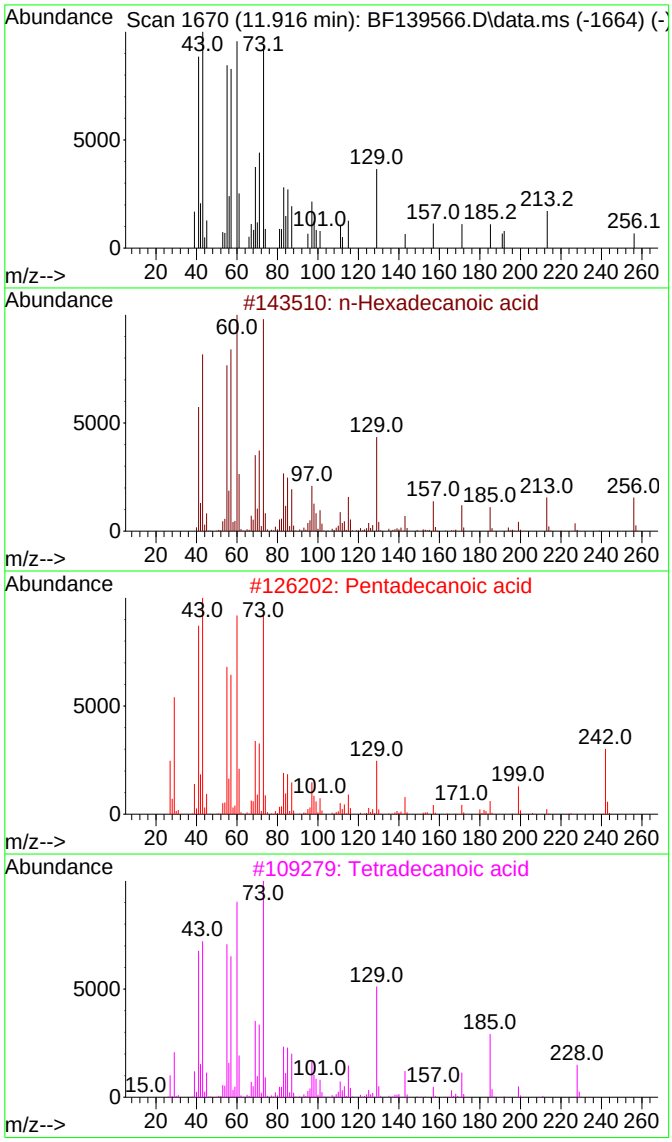
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

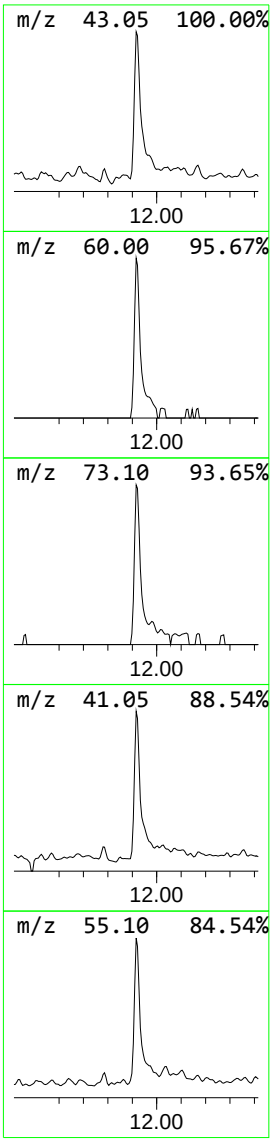
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	2.77 ng	59357	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	59





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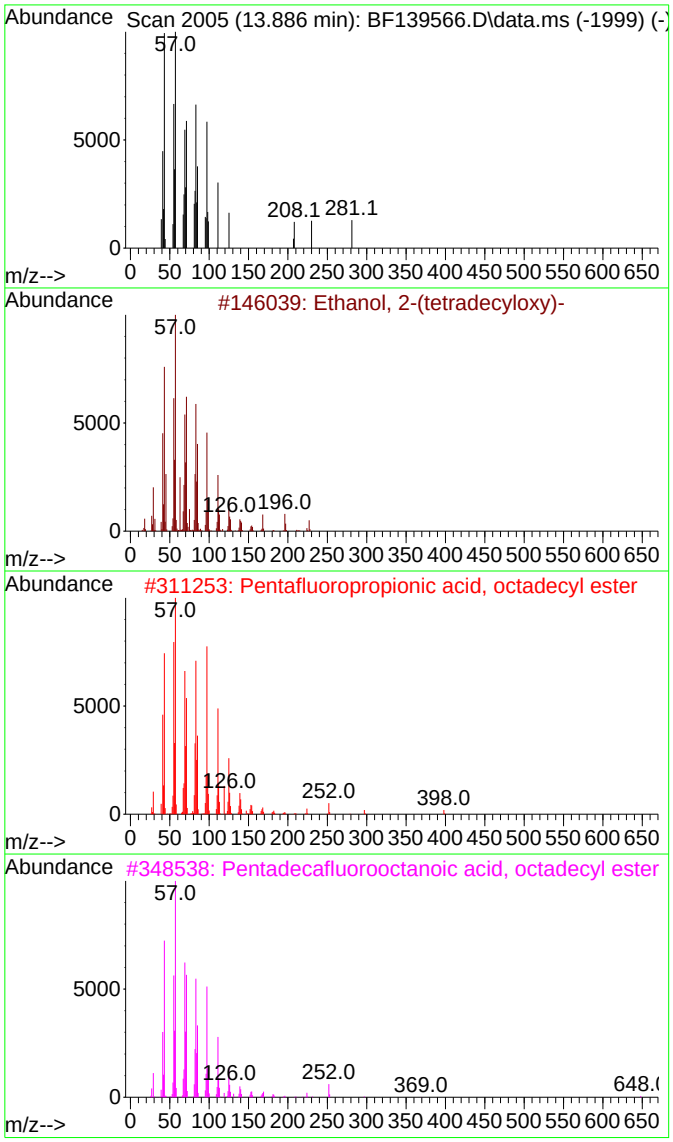
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

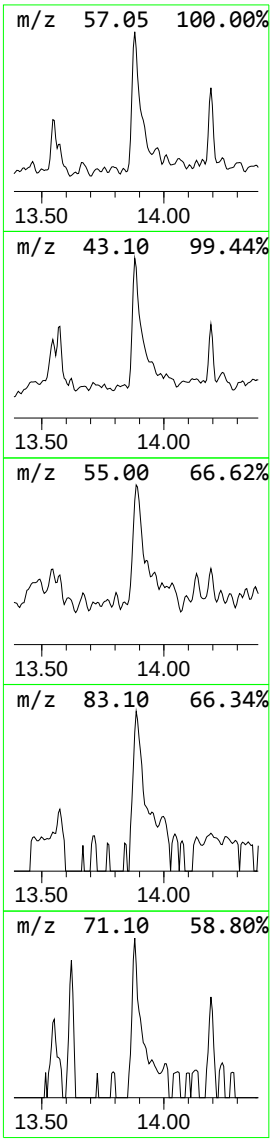
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Ethanol, 2-(tetradecyloxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	3.10 ng	42775	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
2	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	87
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	87
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	83
5	Hexadecyl propyl ether	284	C19H40O	1000406-27-9	83





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...	2.169	200.0	ng	2898970	1	6.875	289944	20.0
(S)-(+)-1,2-Pro...	3.381	6.5	ng	94281	1	6.875	289944	20.0
2-Pentanone, 4-...	5.093	8.8	ng	127287	1	6.875	289944	20.0
1-Phenoxypropan...	8.469	4.1	ng	75843	2	8.157	373265	20.0
unknown10.004	10.004	2.9	ng	58016	3	9.910	405504	20.0
n-Hexadecanoic ...	11.916	2.8	ng	59357	4	11.398	428740	20.0
Ethanol, 2-(tet...	13.886	3.1	ng	42775	5	14.033	275616	20.0