LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052721\
Data File : BF124090.D
Acq On : 27 May 2021 13:42
Operator : JU/CG
Sample : PB136648BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB136648BL

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-BF051421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124090.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.240	20	26	31	rVB	56654	78085	2.78%	0.502%
2	4.498	407	410	417	rBB	34221	36918	1.32%	0.237%
3	5.116	509	515	527	rVB	555005	727895	25.95%	4.678%
4	5.516	577	583	586	rBV	1687858	1839120	65.56%	11.819%
5	5.898	644	648	652	rBB	61715	51077	1.82%	0.328%
6	6.510	746	752	755	rBV	1638640	1788467	63.75%	11.493%
7	6.875	811	814	818	rBV	407657	335195	11.95%	2.154%
8	7.439	904	910	913	rBV	1126405	1273457	45.39%	8.184%
9	8.157	1028	1032	1036	rBV	423891	405512	14.45%	2.606%
10	9.239	1210	1216	1219	rBV	2784134	2381650	84.90%	15.305%
11	9.916	1326	1331	1334	rBV	615182	510317	18.19%	3.279%
12	10.710	1460	1466	1469	rBV	1742731	1692280	60.32%	10.875%
13	11.404	1579	1584	1587	rBV	630282	537521	19.16%	3.454%
14	12.998	1849	1855	1857	rBV	2749145	2805386	100.00%	18.028%
15	13.839	1989	1998	2001	rBV2	20943	28677	1.02%	0.184%
16	13.910	2006	2010	2015	rVB	70403	72394	2.58%	0.465%
17	14.045	2029	2033	2036	rBV	557207	463635	16.53%	2.979%
18	14.821	2160	2165	2172	rBV4	21576	29296	1.04%	0.188%
19	15.168	2220	2224	2230	rBV5	28950	37496	1.34%	0.241%
20	15.533	2278	2286	2290	rBV	292545	391654	13.96%	2.517%
21	16.004	2360	2366	2373	rVB5	26986	44579	1.59%	0.286%
22	16.521	2448	2454	2458	rBV5	16737	30292	1.08%	0.195%

Sum of corrected areas: 15560903

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Misc :
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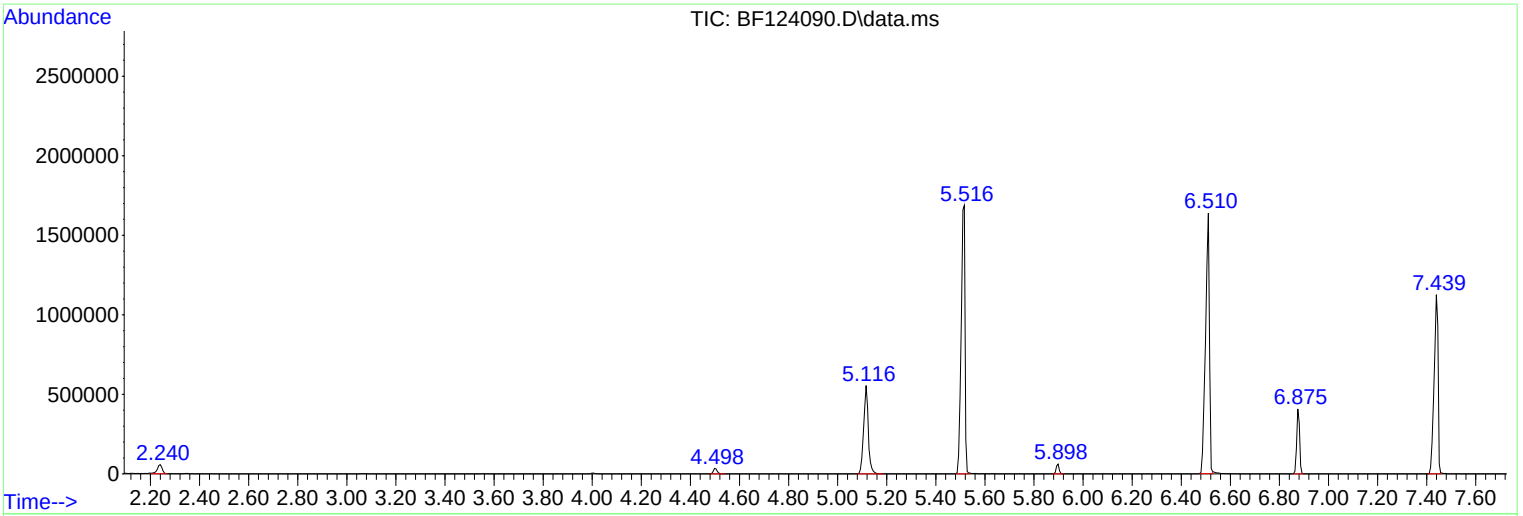
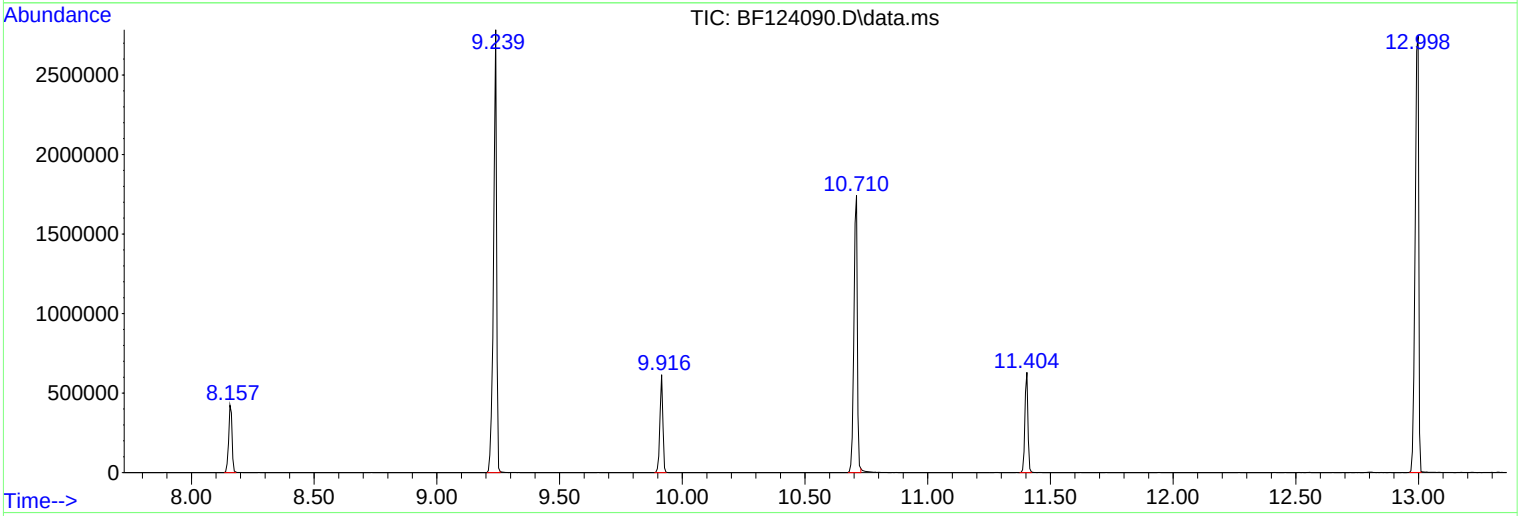
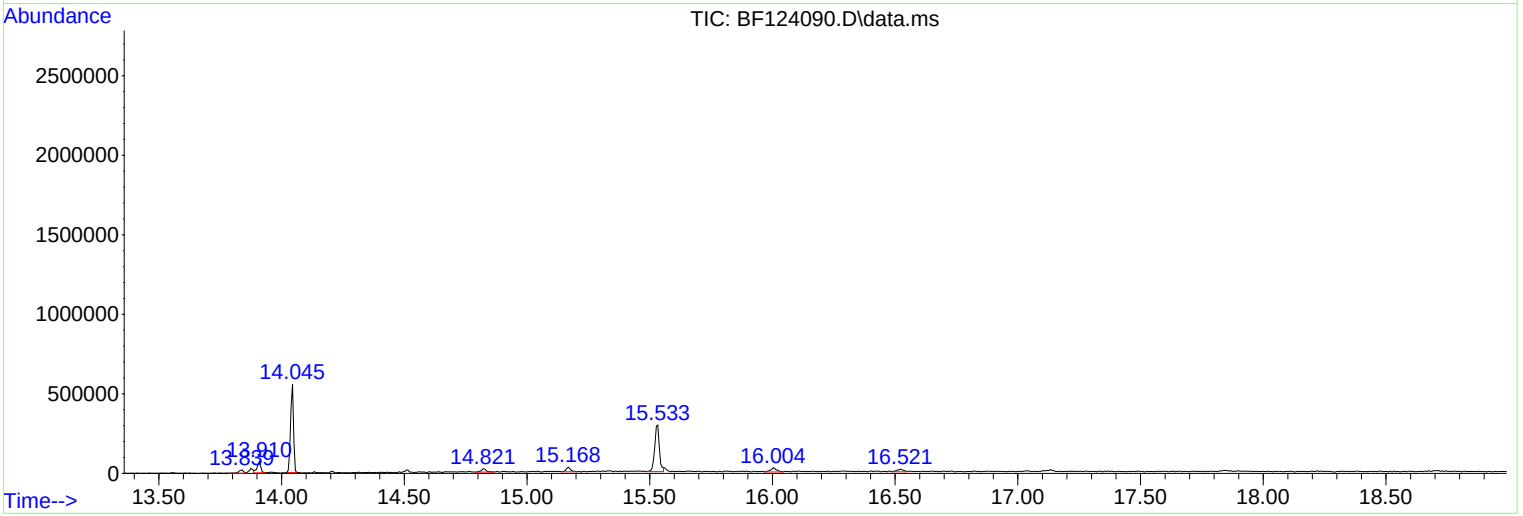
Instrument :
BNA_F
ClientSampleId :
PB136648BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







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Data File : BF124090.D
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Operator : JU/CG
Sample : PB136648BL
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Instrument : BNA_F
ClientSampleId : PB136648BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

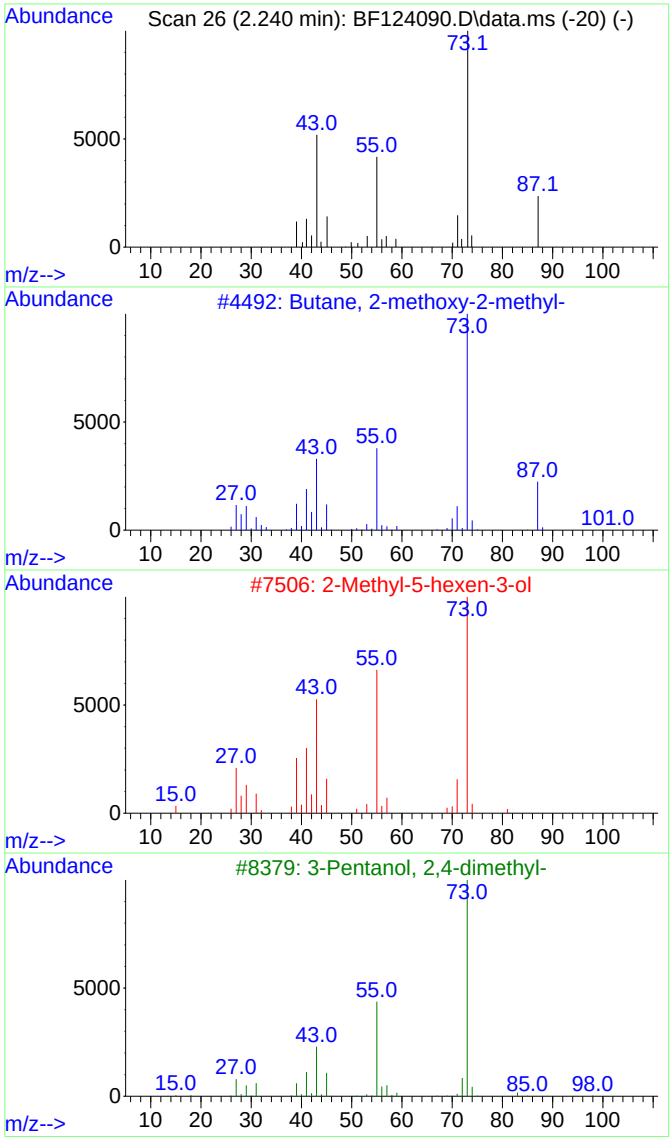
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

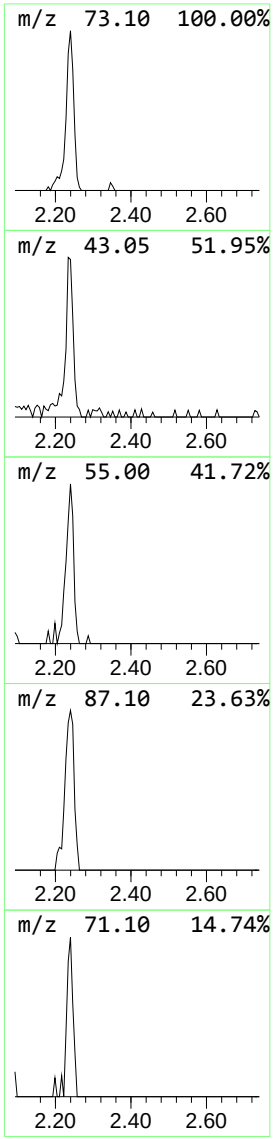
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.240	4.66 ng	78085	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	64
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	32
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	28
4	1-Butanol, 2,2-dimethyl-	102	C6H14O	001185-33-7	12
5	1-Butanol, 2-methyl-, acetate	130	C7H14O2	000624-41-9	10





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Operator : JU/CG
Sample : PB136648BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB136648BL

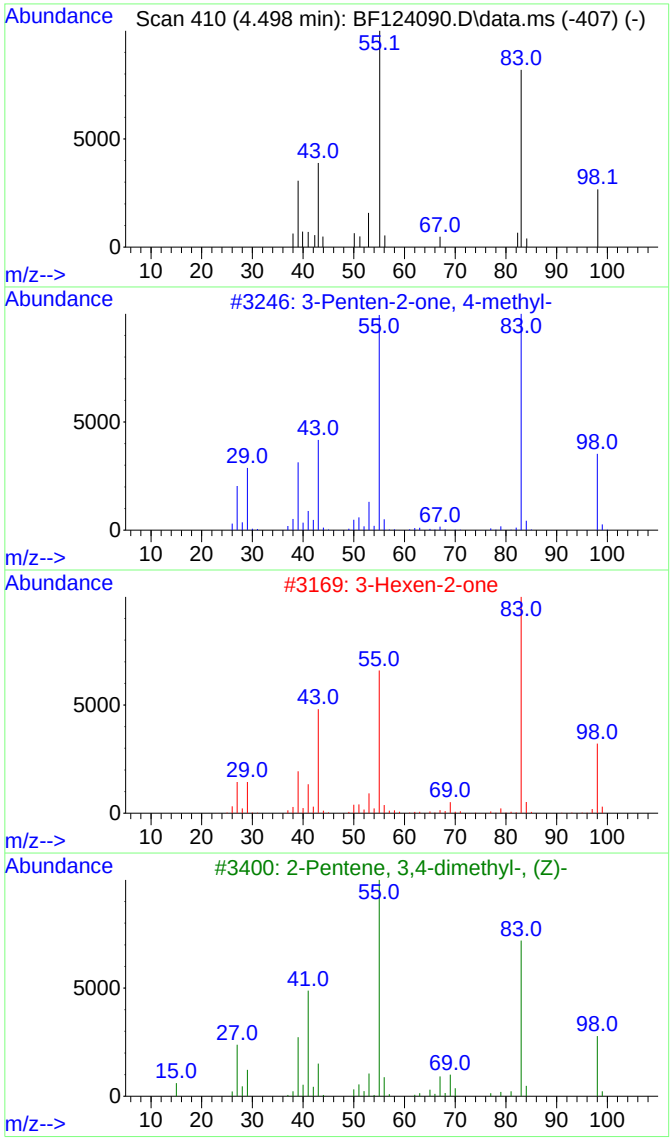
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

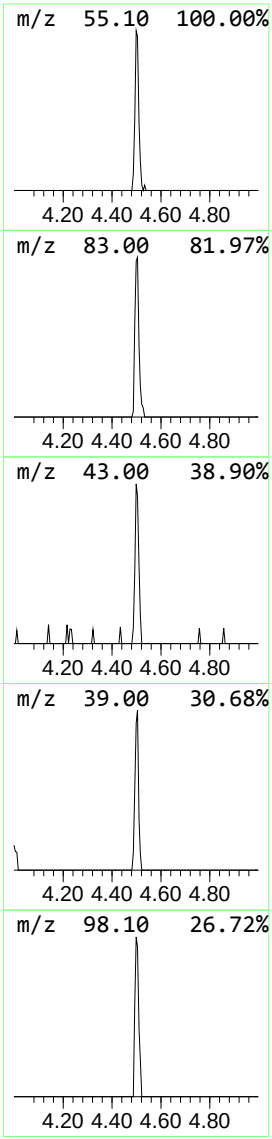
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.498	2.20 ng	36918	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	87
2	3-Hexen-2-one	98	C6H10O	000763-93-9	80
3	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	72
5	2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052721\
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Operator : JU/CG
Sample : PB136648BL
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ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB136648BL

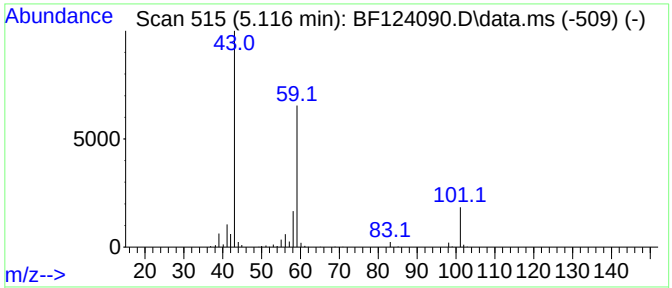
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

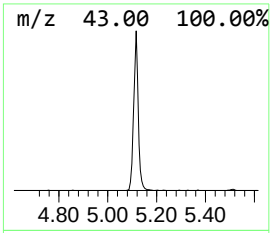
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

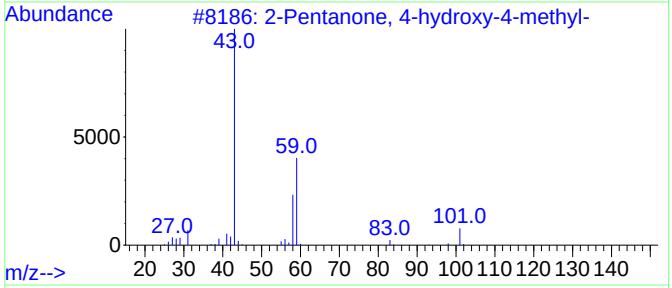
****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

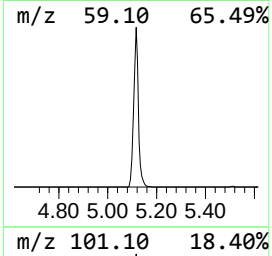
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	43.43 ng	727895	1,4-Dichlorobenzene-d4	6.875

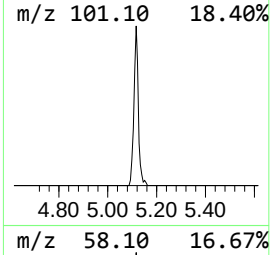
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	32
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28

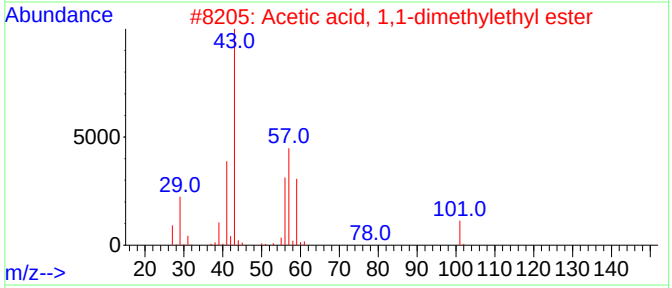


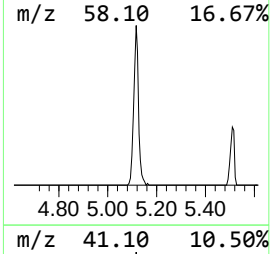


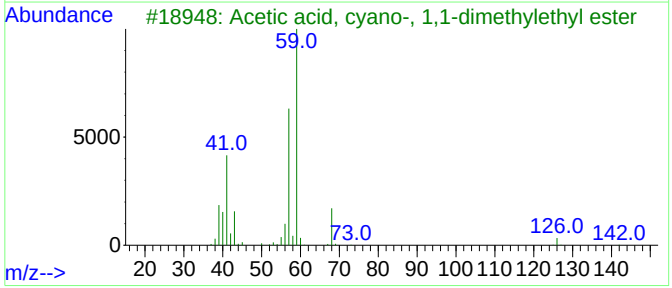


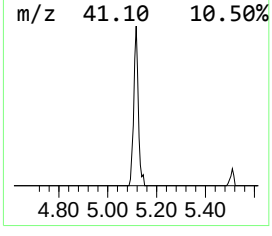












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Instrument :
BNA_F
ClientSampleId :
PB136648BL

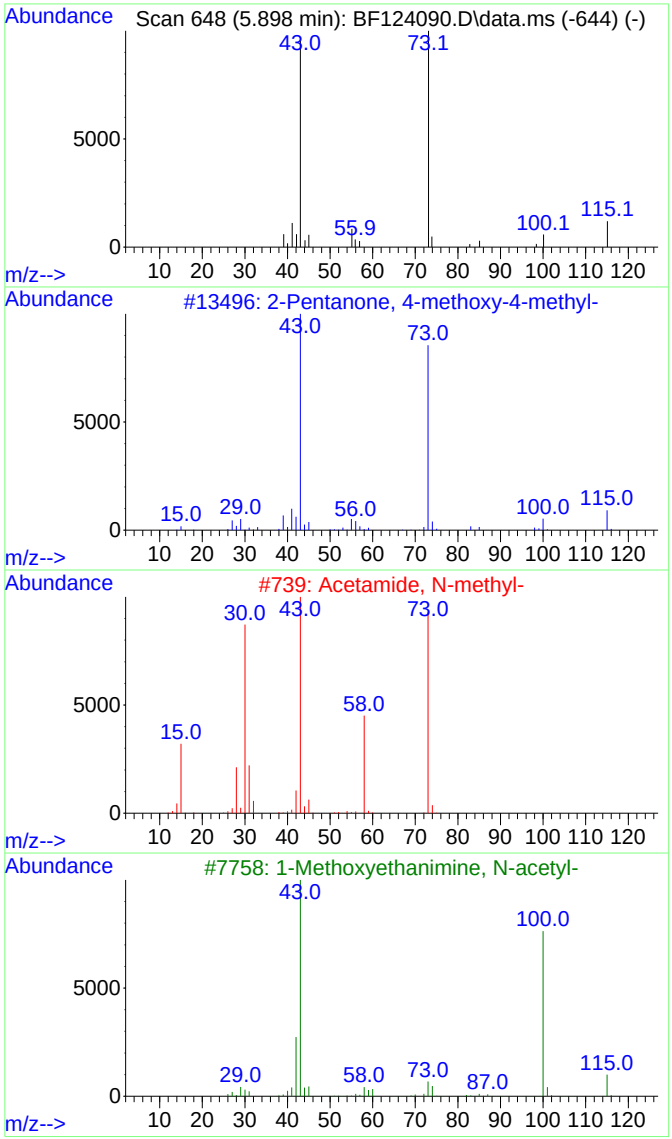
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

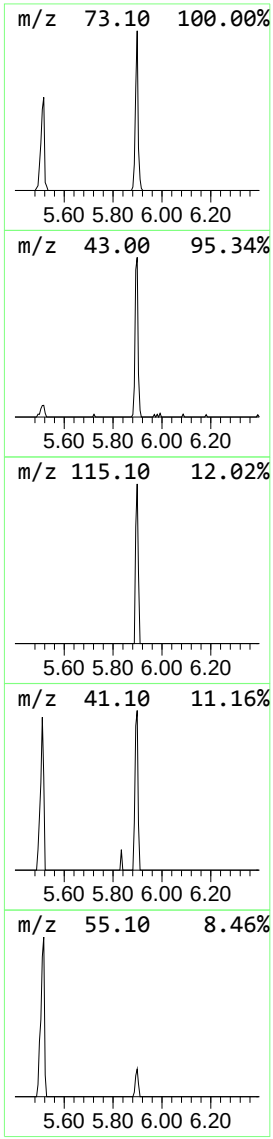
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.898	3.05 ng	51077	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
3	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	9
4	Acetamide, N-butyl-	115	C6H13NO	001119-49-9	9
5	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	9





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Sample : PB136648BL
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Instrument :
BNA_F
ClientSampleId :
PB136648BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
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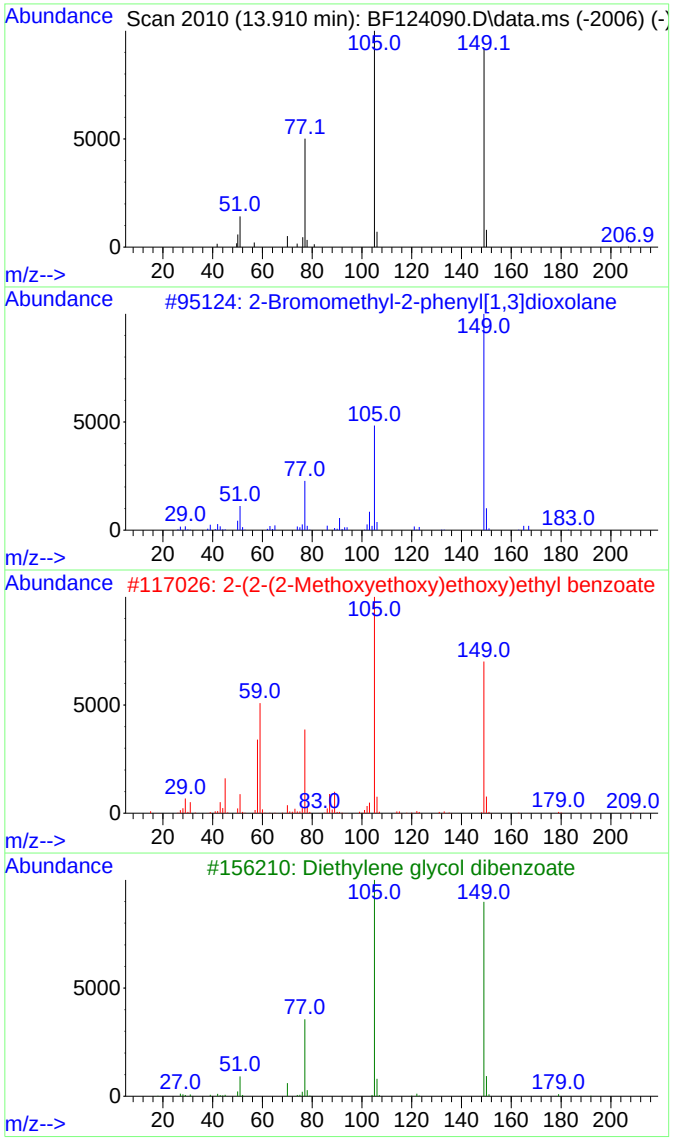
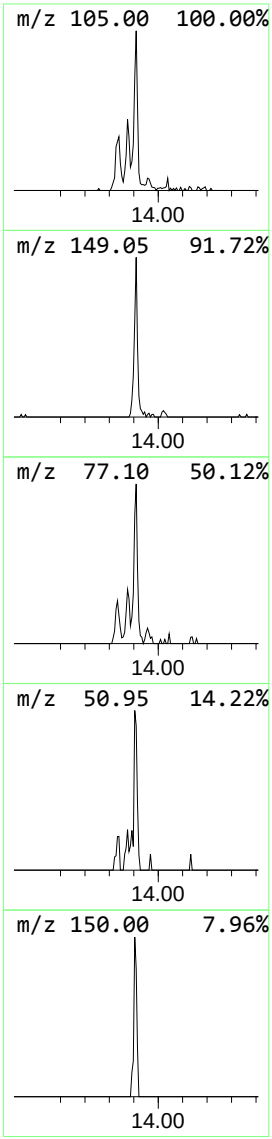
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Bromomethyl-2-phenyl[1,3]... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	3.12 ng	72394	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromomethyl-2-phenyl[1,3]dioxo...	242	C10H11BrO2	003418-21-1	74
2	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	74
3	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	56
4	Benzoyl bromide	184	C7H5BrO	000618-32-6	38
5	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	38





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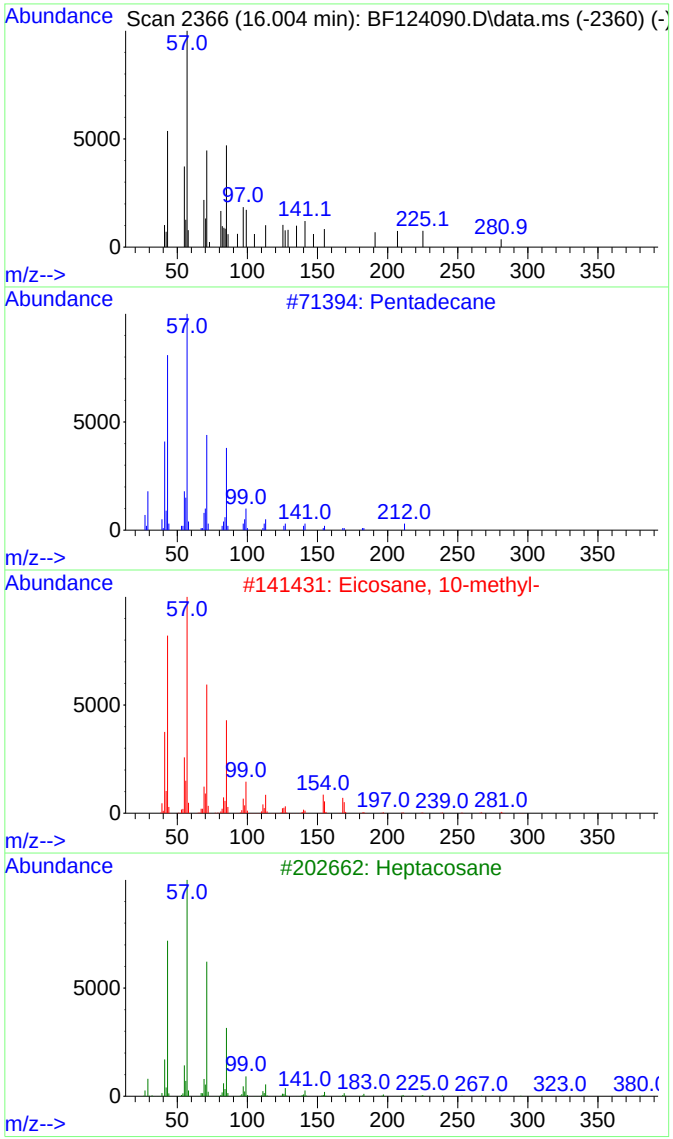
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

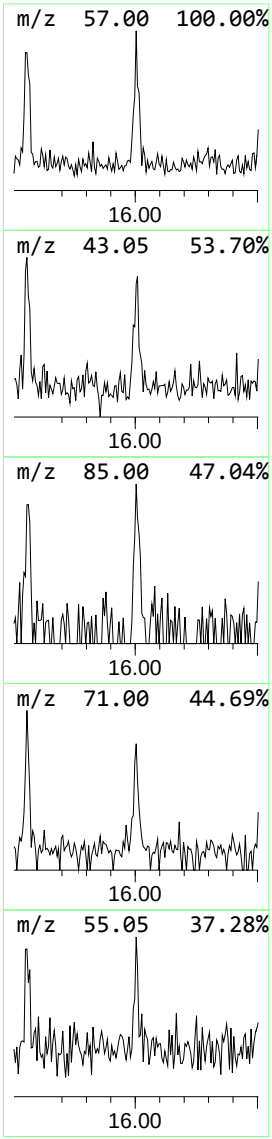
****

Peak Number 6 Pentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.003	2.28 ng	44579	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	59
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	53
3	Heptacosane	380	C27H56	000593-49-7	53
4	Tridecane, 2-methyl-	198	C14H30	001560-96-9	53
5	Heneicosane	296	C21H44	000629-94-7	53





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.240	4.7	ng	78085	1	6.875	335195	20.0
3-Penten-2-one,...	4.498	2.2	ng	36918	1	6.875	335195	20.0
2-Pentanone, 4-...	5.116	43.4	ng	727895	1	6.875	335195	20.0
2-Pentanone, 4-...	5.898	3.0	ng	51077	1	6.875	335195	20.0
2-Bromomethyl-2...	13.910	3.1	ng	72394	5	14.045	463635	20.0
Pentadecane	16.003	2.3	ng	44579	6	15.533	391654	20.0