LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100121\
Data File : BF125754.D
Acq On : 1 Oct 2021 16:07
Operator : JU/CG
Sample : M4002-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 290-359

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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-BF092421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125754.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	10	18	28	rVB	1492908	1900719	32.06%	4.801%
2	2.299	30	36	42	rBV	67672	86430	1.46%	0.218%
3	3.640	259	264	273	rBV	91575	128720	2.17%	0.325%
4	4.510	403	412	416	rBV	4086712	5928769	100.00%	14.974%
5	5.116	508	515	518	rBV	2012255	2388510	40.29%	6.033%
6	5.504	577	581	585	rBV	2806726	2809784	47.39%	7.097%
7	6.510	746	752	755	rBV	3375738	3527558	59.50%	8.909%
8	6.887	812	816	819	rBV	1463092	1131639	19.09%	2.858%
9	7.204	866	870	873	rBV	192888	158670	2.68%	0.401%
10	7.445	906	911	914	rBV	2929968	2626443	44.30%	6.634%
11	8.063	1013	1016	1028	rBV	454910	447281	7.54%	1.130%
12	8.169	1030	1034	1037	rBV	1828849	1564431	26.39%	3.951%
13	9.245	1212	1217	1220	rBV	5509363	5166051	87.14%	13.048%
14	9.922	1328	1332	1343	rBV	2161507	1778670	30.00%	4.492%
15	10.704	1462	1465	1476	rBV	1086603	999100	16.85%	2.523%
16	11.404	1580	1584	1588	rBV	1976509	1739924	29.35%	4.394%
17	12.992	1849	1854	1857	rBV	5149960	4724081	79.68%	11.931%
18	13.892	2003	2007	2016	rBV2	42744	96628	1.63%	0.244%
19	14.039	2028	2032	2040	rVB	1176618	1146452	19.34%	2.896%
20	15.515	2278	2283	2295	rBV	940169	1243593	20.98%	3.141%

Sum of corrected areas: 39593453

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Misc :
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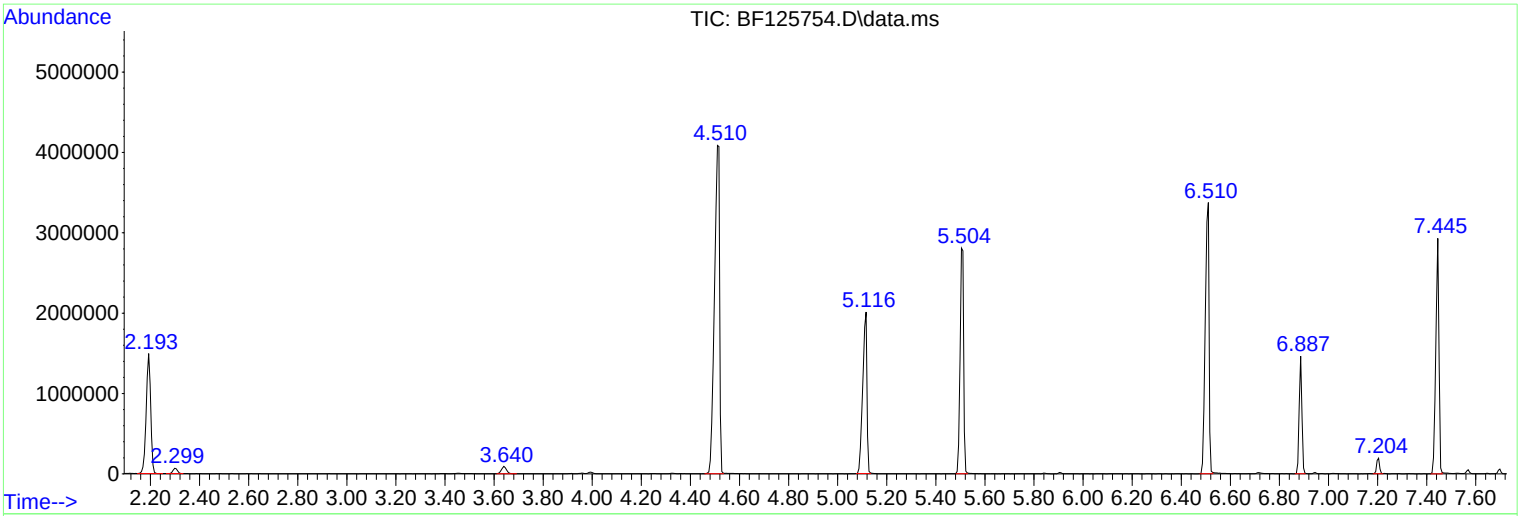
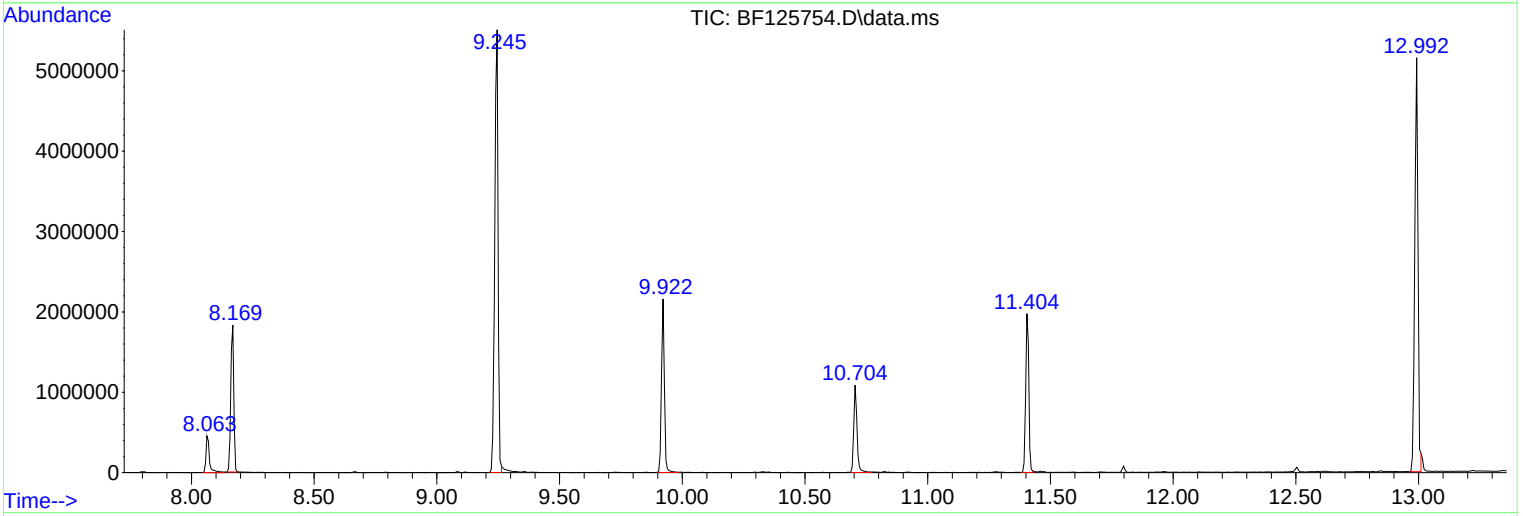
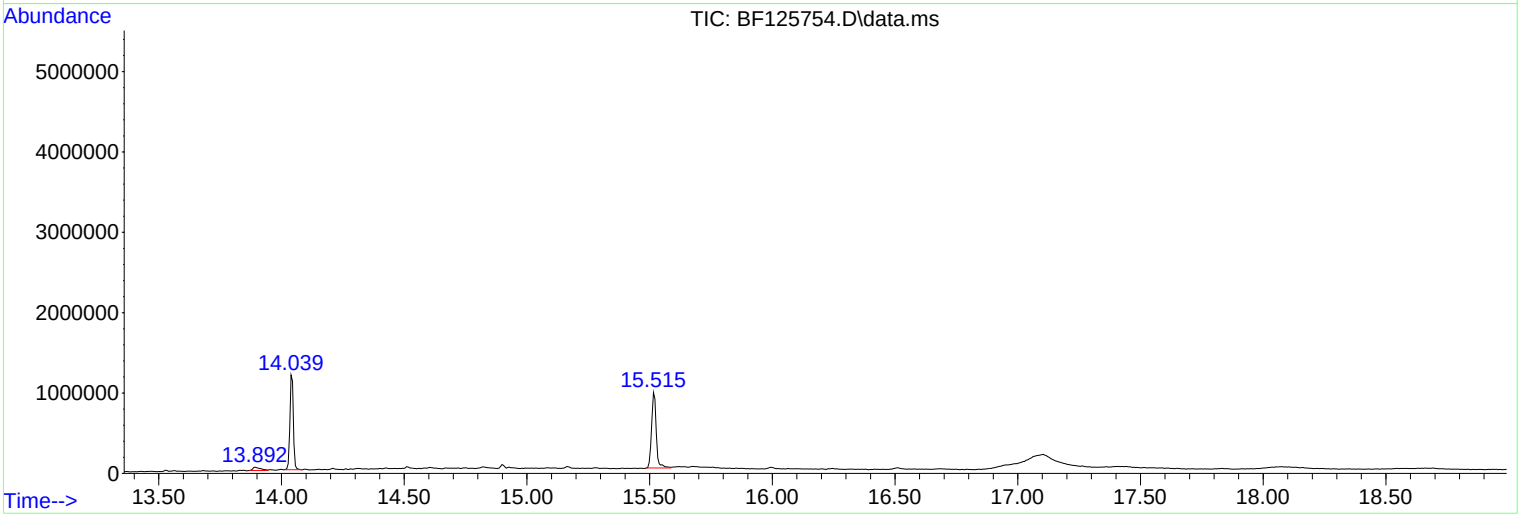
Instrument :
BNA_F
ClientSampleId :
290-359

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.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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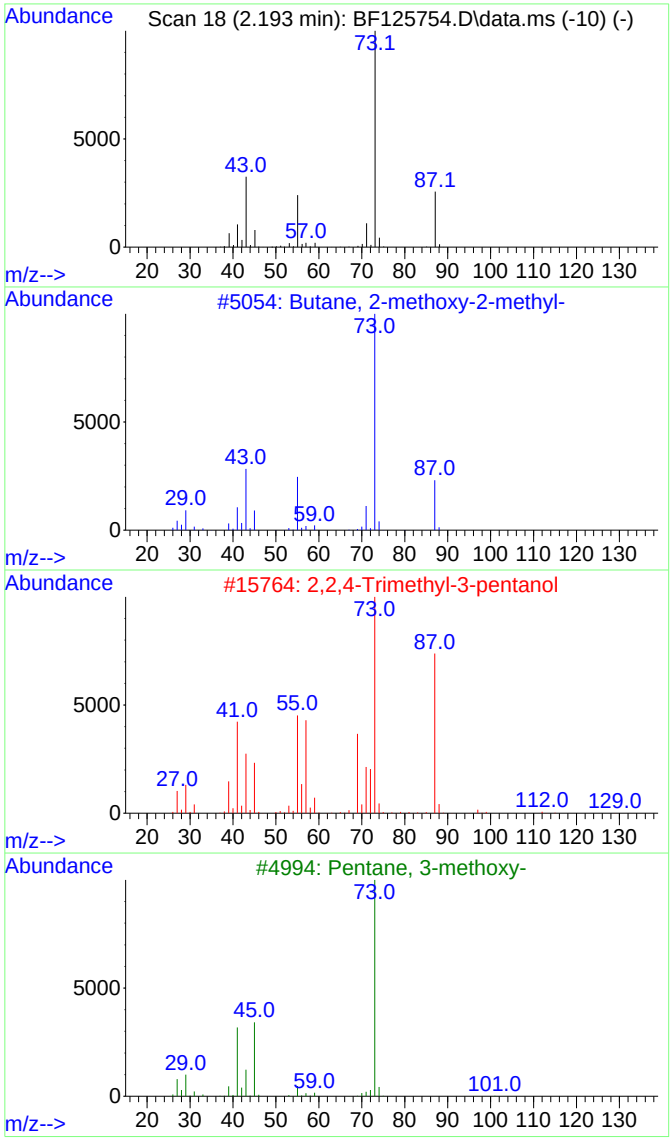
TIC Integration Parameters: LSCINT.P

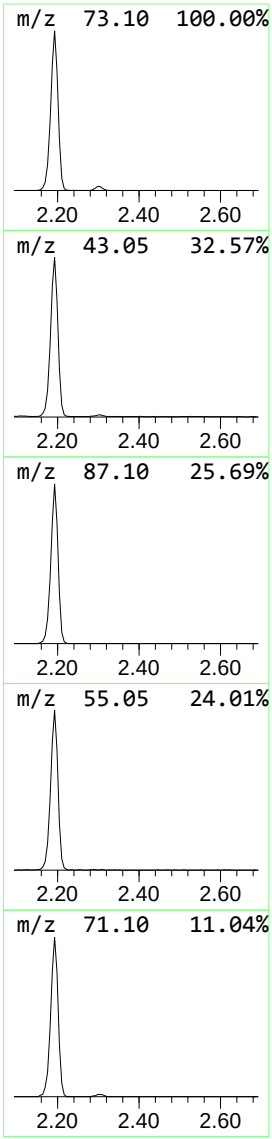
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	33.59 ng	1900720	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	43
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





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Instrument : BNA_F
ClientSampleId : 290-359

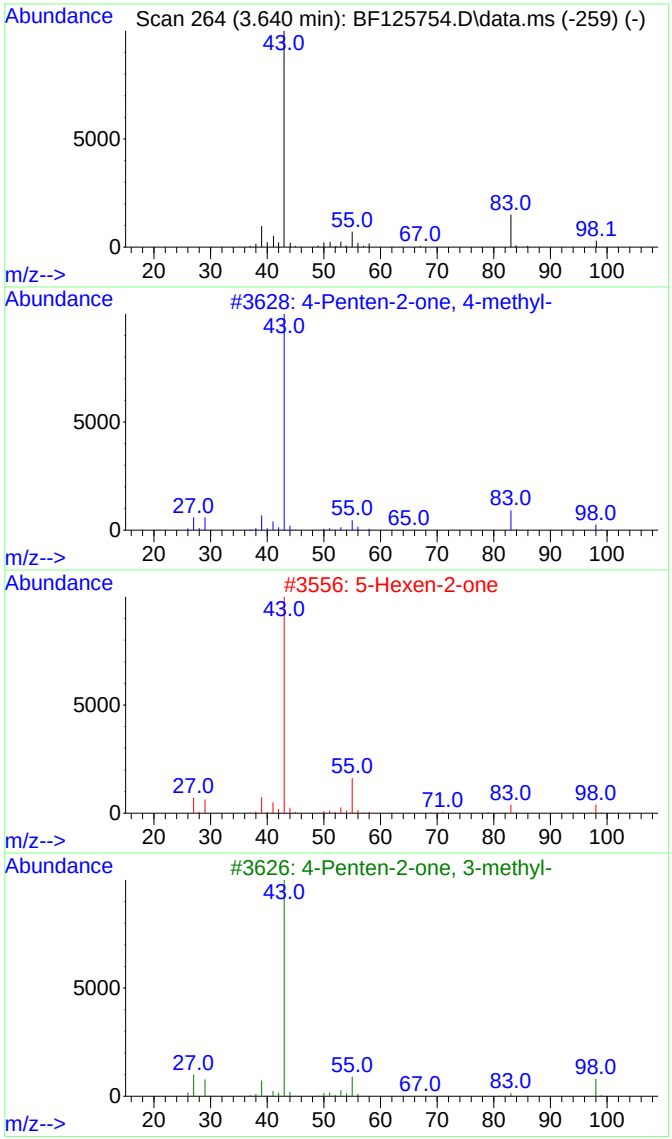
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

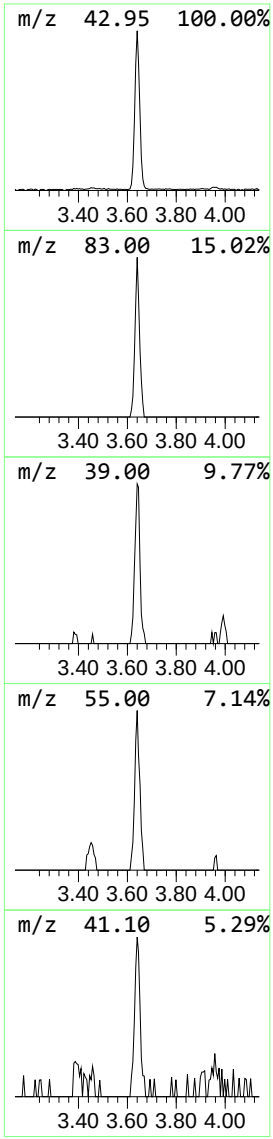
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.640	2.27 ng	128720	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	80
2	5-Hexen-2-one	98	C6H10O	000109-49-9	43
3	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	38
4	2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	12
5	Isoxazole, 5-methyl-	83	C4H5NO	005765-44-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100121\
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Operator : JU/CG
Sample : M4002-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 290-359

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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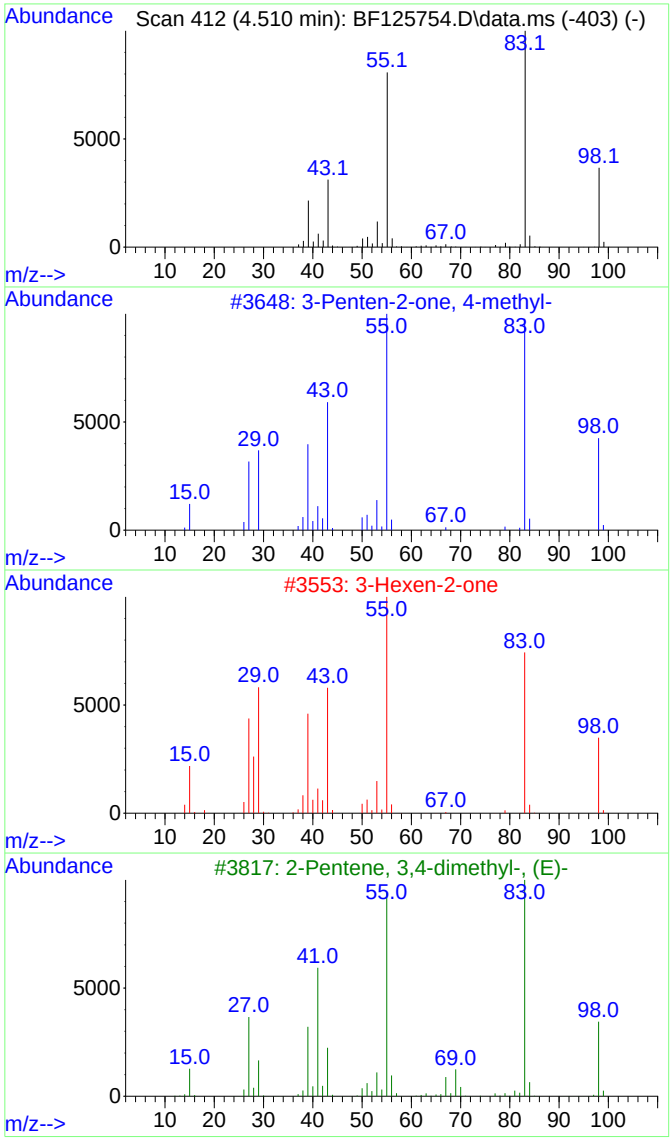
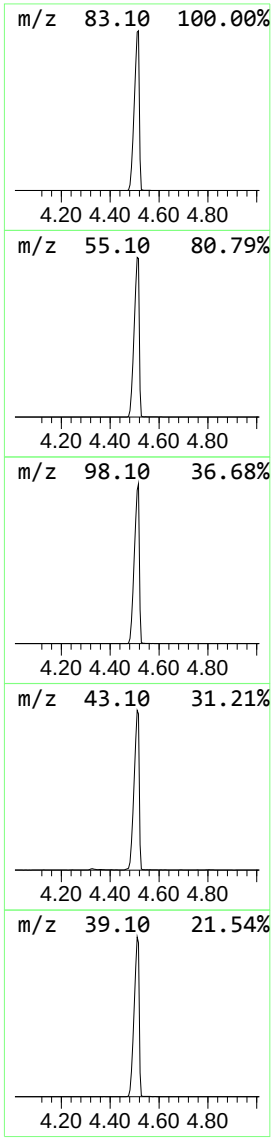
****

Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.510	104.78 ng	5928770	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-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	78





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Sample : M4002-01
Misc :
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Instrument : BNA_F
ClientSampleId : 290-359

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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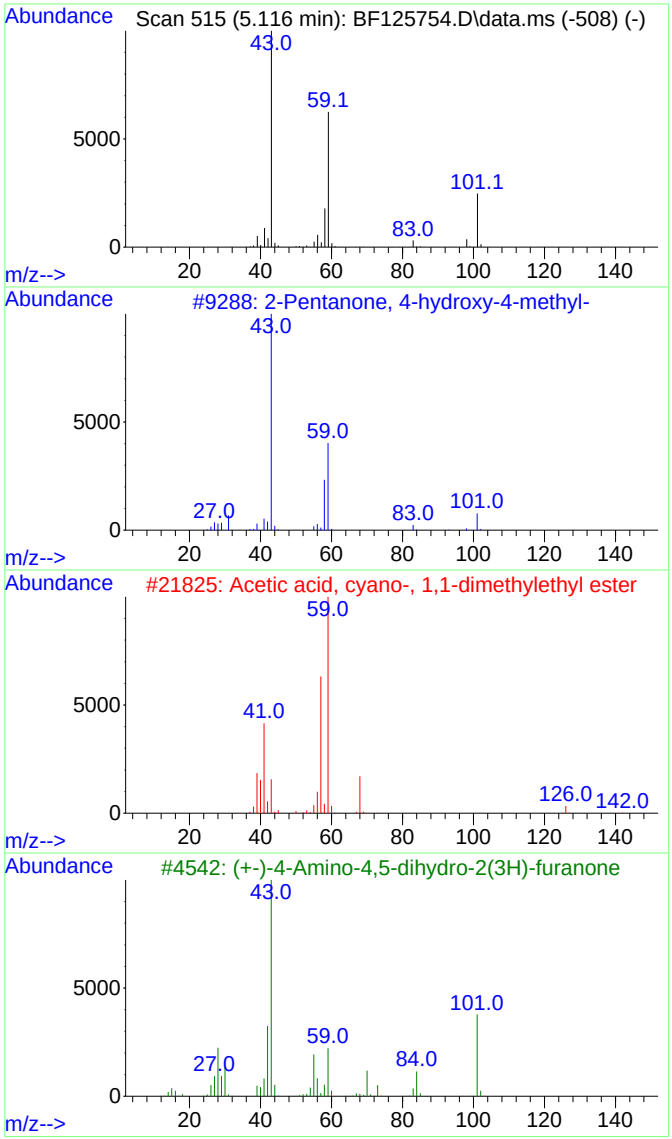
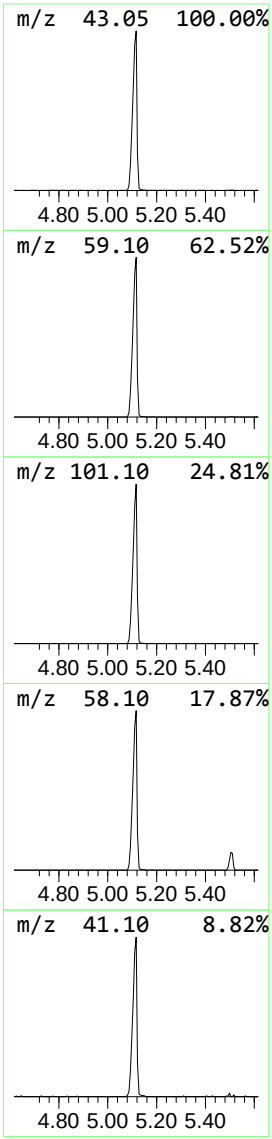
****
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	42.21 ng	2388510	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	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4	Acetone	58	C3H6O	000067-64-1	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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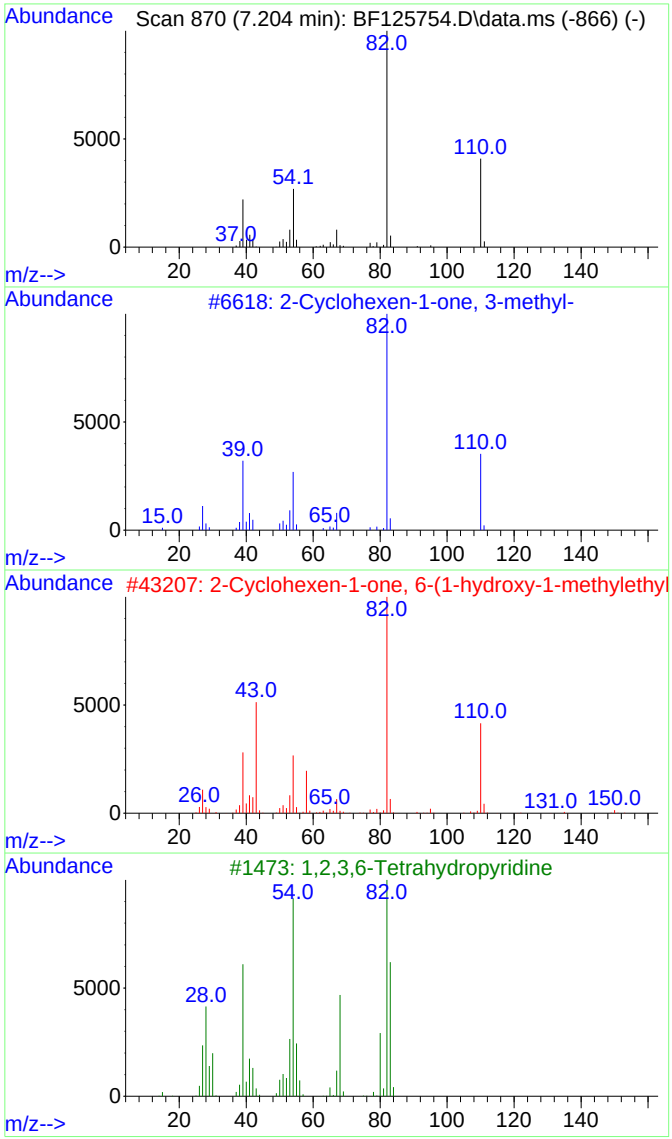
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

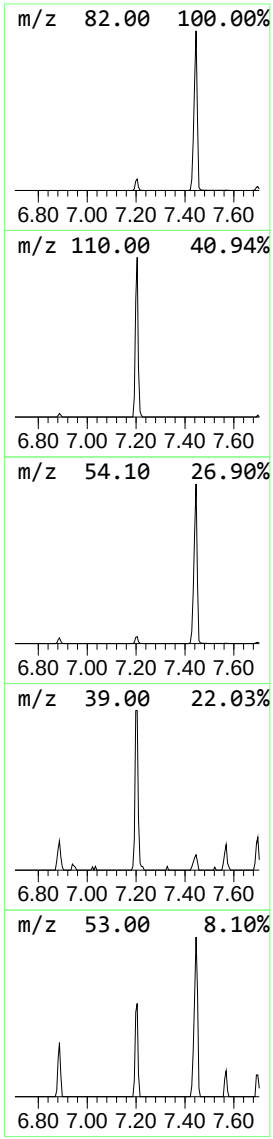
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.204	2.80 ng	158670	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	91
2	2-Cyclohexen-1-one, 6-(1-hydroxy...	168	C10H16O2	087791-00-2	64
3	1,2,3,6-Tetrahydropyridine	83	C5H9N	000694-05-3	53
4	Betazole	111	C5H9N3	000105-20-4	47
5	1H-Pyrazole, 1-methyl-	82	C4H6N2	000930-36-9	40





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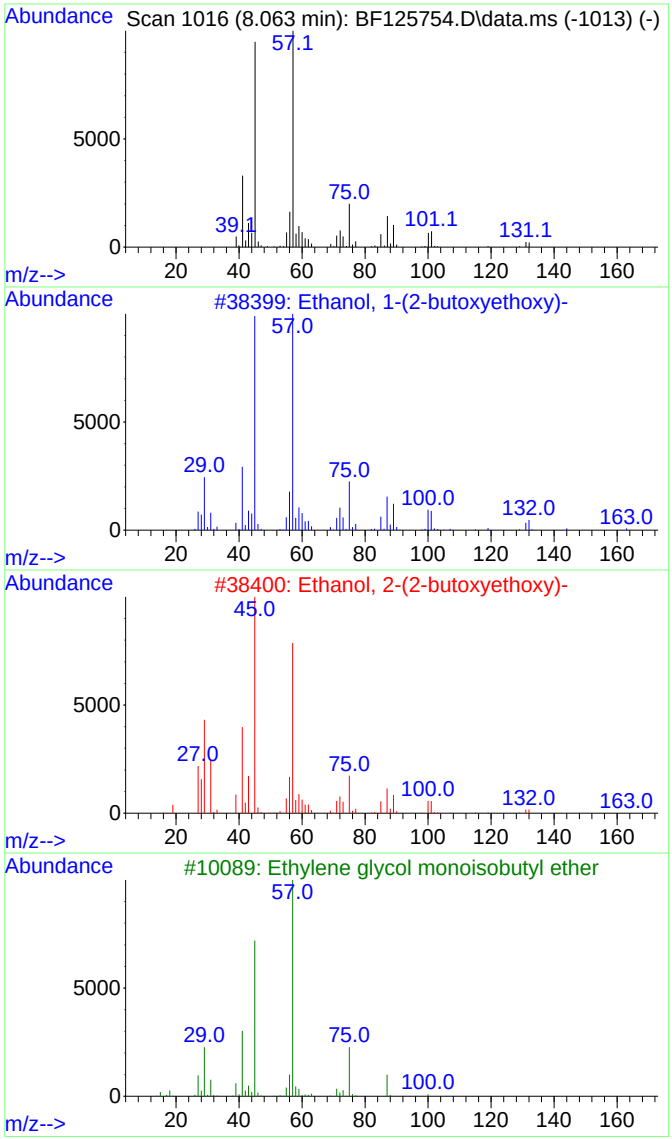
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

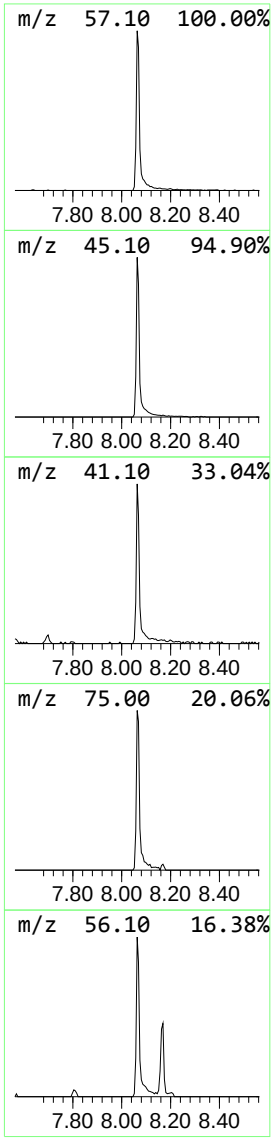
****

Peak Number 6 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.063	5.72 ng	447281	Naphthalene-d8	8.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5	Di-sec-Butyl ether	130	C8H18O	006863-58-7	50





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.193	33.6	ng	1900720	1	6.887	1131640	20.0
4-Penten-2-one,...	3.640	2.3	ng	128720	1	6.887	1131640	20.0
3-Penten-2-one,...	4.510	104.8	ng	5928770	1	6.887	1131640	20.0
2-Pentanone, 4-...	5.116	42.2	ng	2388510	1	6.887	1131640	20.0
2-Cyclohexen-1-...	7.204	2.8	ng	158670	1	6.887	1131640	20.0
Ethanol, 1-(2-b...	8.063	5.7	ng	447281	2	8.169	1564430	20.0