LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061621\
Data File : BF124344.D
Acq On : 16 Jun 2021 14:00
Operator : JU/CG
Sample : M2691-02 10X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-VNJ-208

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-BF060321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124344.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.751	108	113	122	rBB2	66352	103839	1.11%	0.765%
2	3.387	214	221	233	rBV	141753	262540	2.80%	1.933%
3	4.398	377	393	395	rBV	3529609	9388705	100.00%	69.141%
4	6.781	795	798	802	rBV	271333	223508	2.38%	1.646%
5	6.916	818	821	823	rBV	181067	137621	1.47%	1.013%
6	7.475	912	916	919	rBV	405032	321433	3.42%	2.367%
7	8.069	1013	1017	1019	rBV	356017	295608	3.15%	2.177%
8	9.139	1197	1199	1205	rVB	147292	111142	1.18%	0.818%
9	9.821	1312	1315	1318	rVB	362493	280778	2.99%	2.068%
10	10.610	1446	1449	1455	rBV3	116083	116646	1.24%	0.859%
11	11.310	1564	1568	1570	rBV	431944	372628	3.97%	2.744%
12	11.333	1570	1572	1575	rVV	563365	433659	4.62%	3.194%
13	12.527	1771	1775	1778	rBV	437061	355417	3.79%	2.617%
14	12.757	1811	1814	1818	rVB	195767	185891	1.98%	1.369%
15	12.892	1830	1837	1845	rVB2	128691	145784	1.55%	1.074%
16	13.957	2012	2018	2020	rBV2	316044	408811	4.35%	3.011%
17	13.980	2020	2022	2025	rVB	142834	114735	1.22%	0.845%
18	14.992	2190	2194	2197	rBV	109941	144979	1.54%	1.068%
19	15.415	2261	2266	2277	rVB3	105444	175395	1.87%	1.292%

Sum of corrected areas: 13579119

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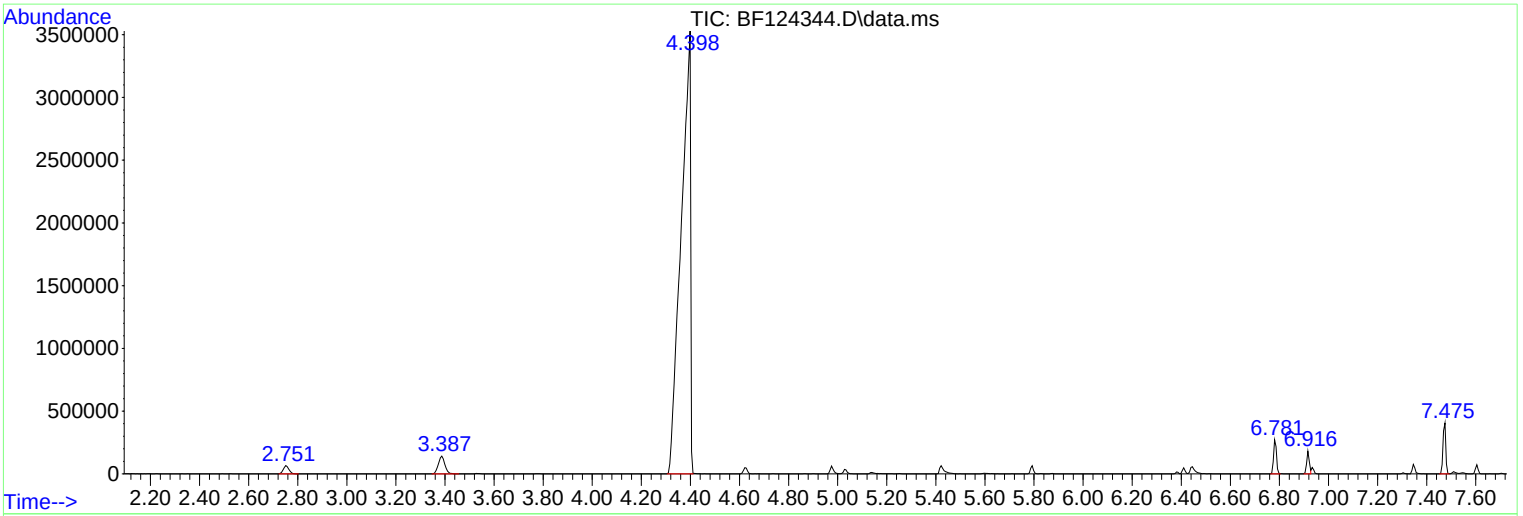
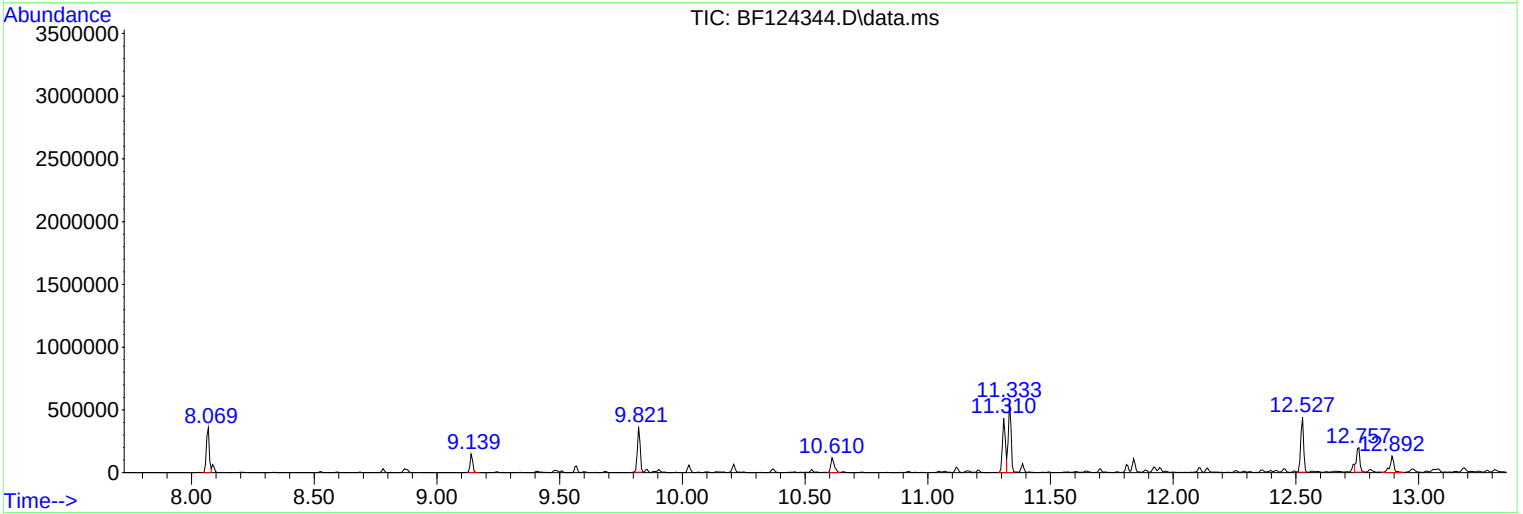
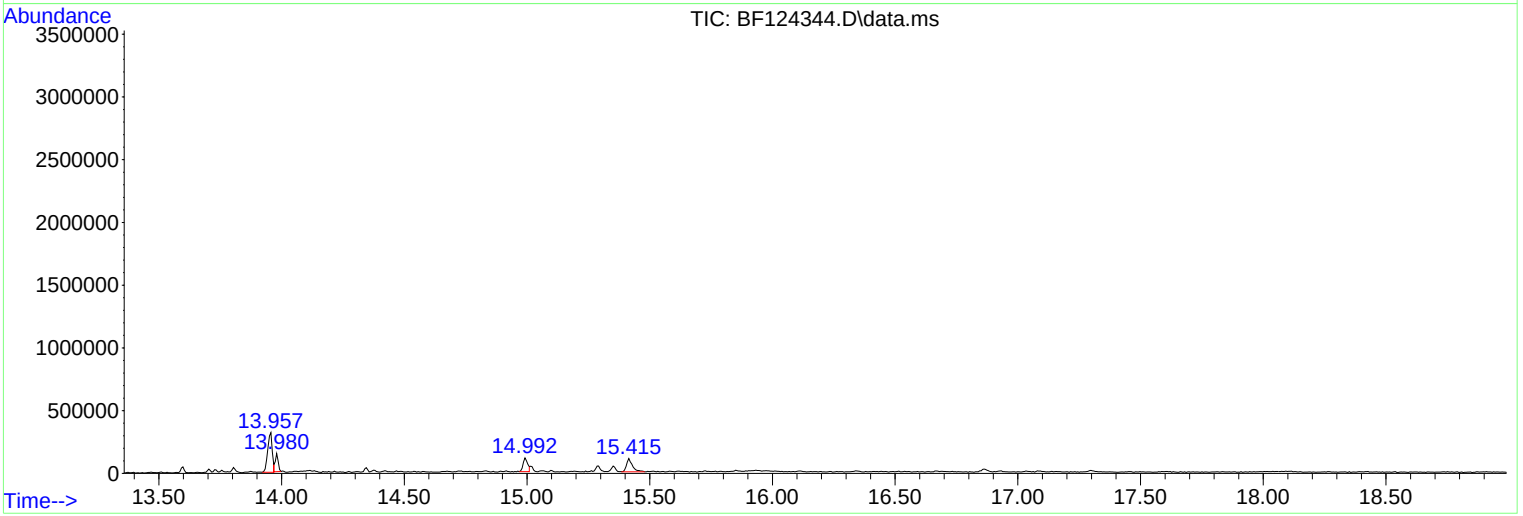
BNA_F
ClientSampleId :
RO-VNJ-208

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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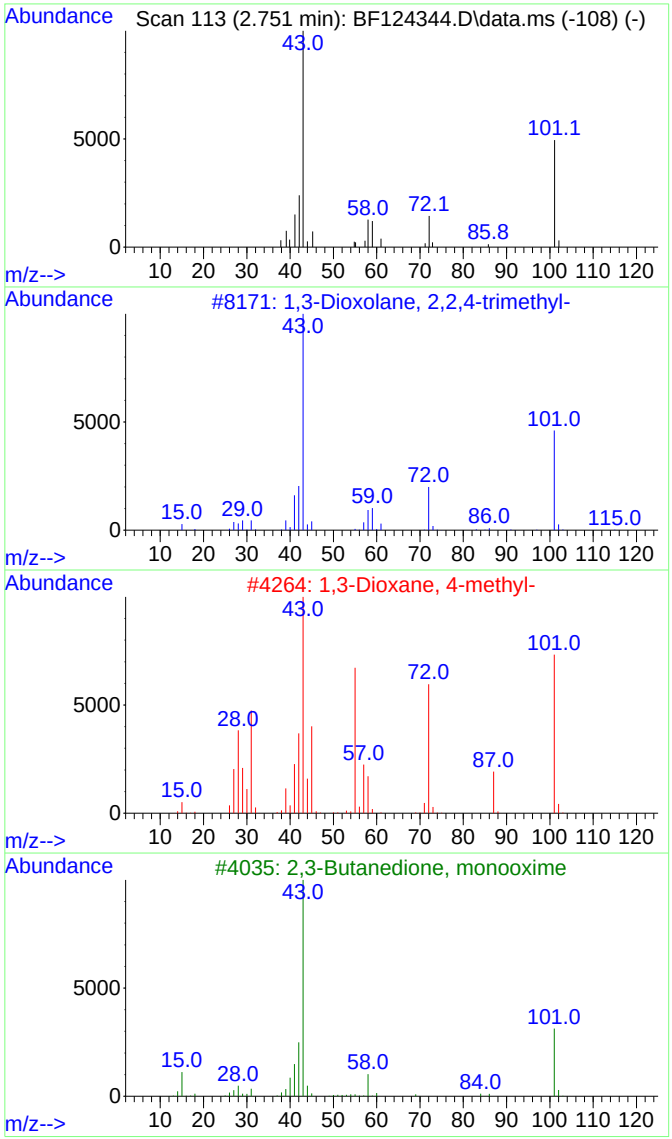
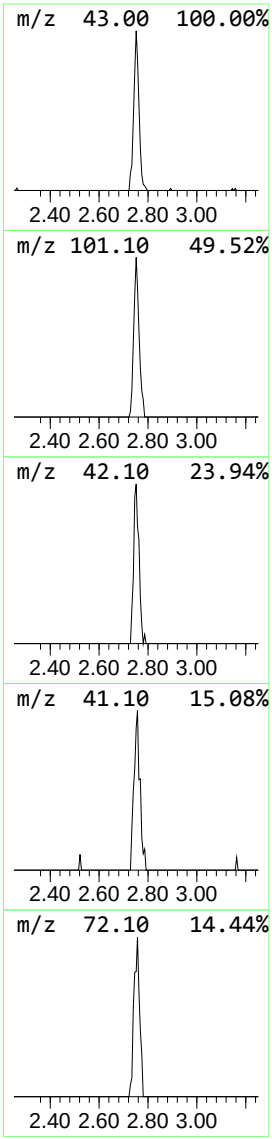
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.751	9.29 ng	103839	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	78
2	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	53
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	36
4	Ethanethioic acid, S-(dihydro-2,...	174	C6H6O4S	006953-60-2	12
5	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	9





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Instrument :
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ClientSampleId :
RO-VNJ-208

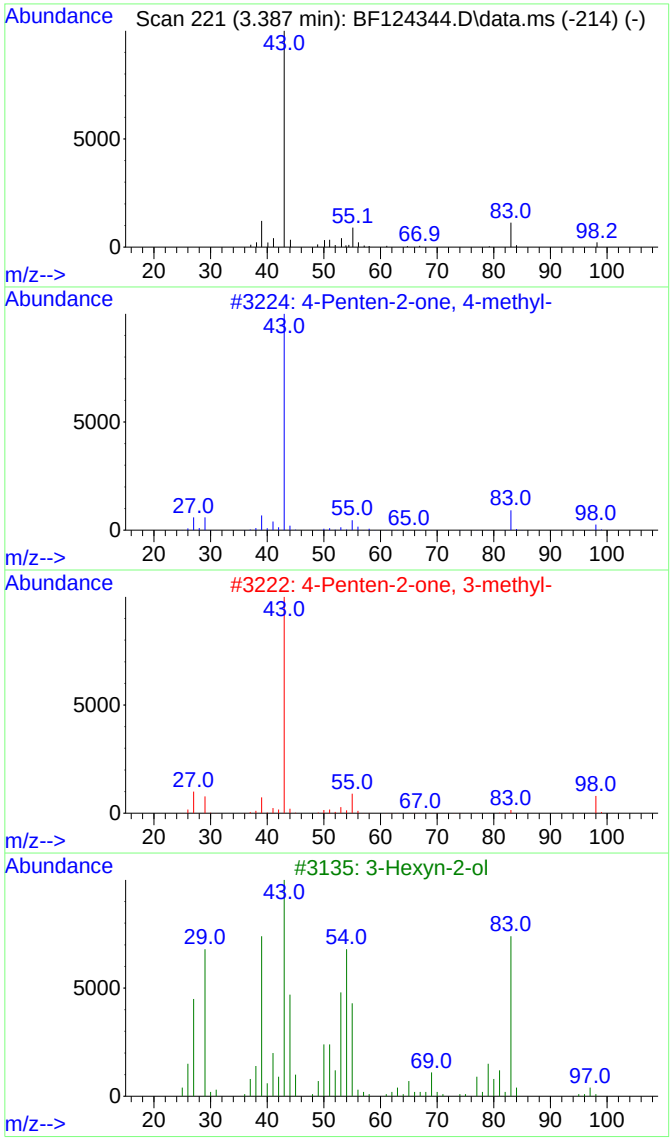
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

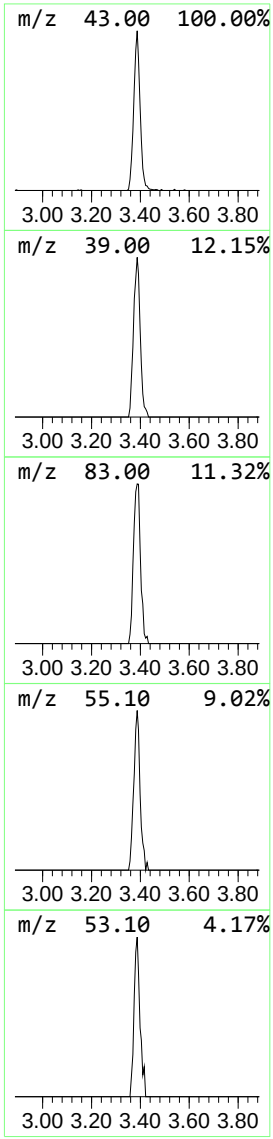
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.387	23.49 ng	262540	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	53
2	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	50
3	3-Hexyn-2-ol	98	C6H10O	000109-50-2	12
4	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Data File : BF124344.D
Acq On : 16 Jun 2021 14:00
Operator : JU/CG
Sample : M2691-02 10X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-VNJ-208

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

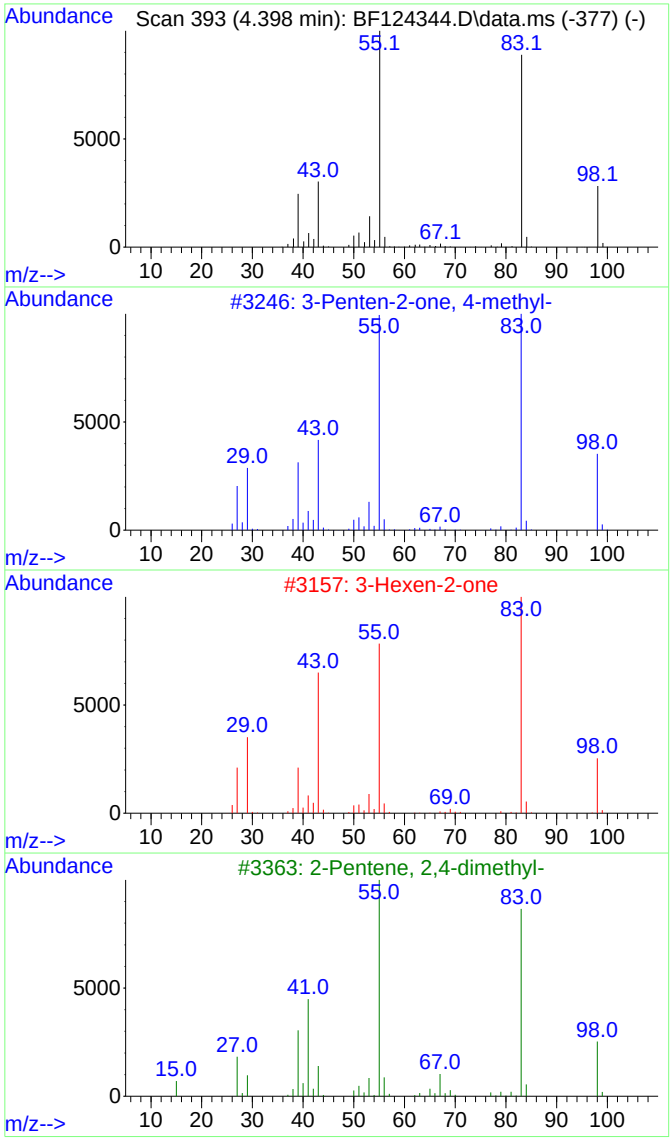
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

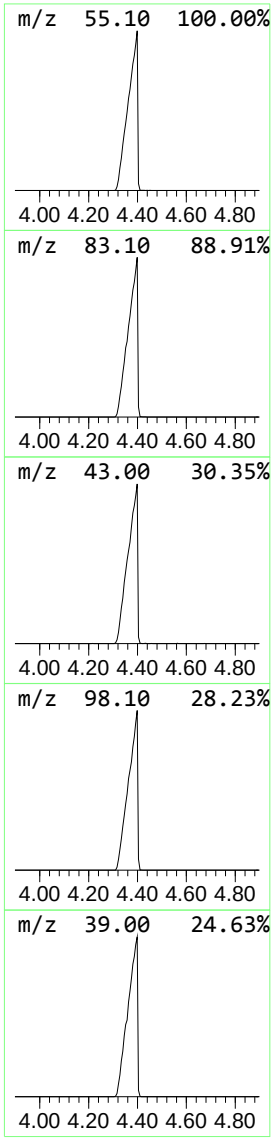
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.398	840.12 ng	9388710	1,4-Dichlorobenzene-d4	6.781

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





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Instrument : BNA_F
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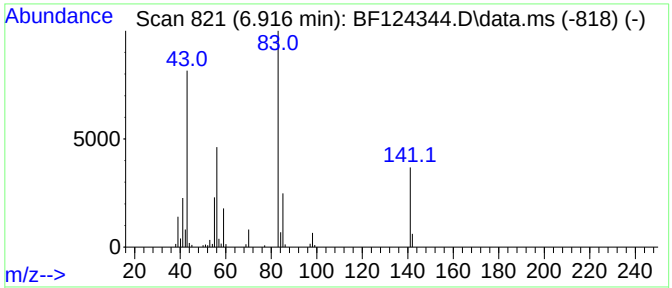
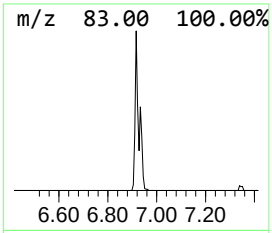
****

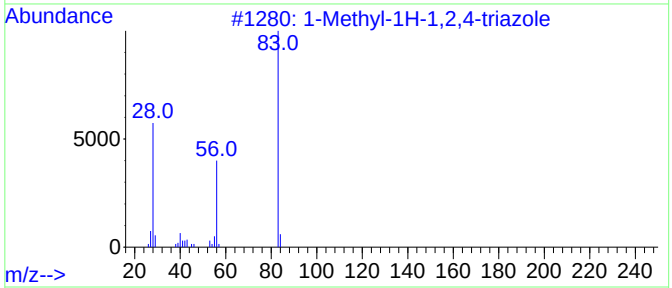
Peak Number 4 unknown6.916 Concentration Rank 4

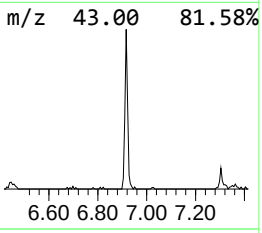
R.T.	EstConc	Area	Relative to ISTD	R.T.
6.916	12.31 ng	137621	1,4-Dichlorobenzene-d4	6.781

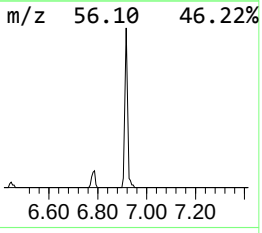
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	47
2	Tetrahydropyrrolo[2,1-c][1,4]oxa...	141	C7H11NO2	101250-37-7	37
3	Propane-1,3-diyl bis((E)-2-methy...	240	C13H20O4	1000373-72-9	23
4	1-Pentene, 4-methyl-	84	C6H12	000691-37-2	10
5	(Trimethylsilyl)acetylene	98	C5H10Si	001066-54-2	9

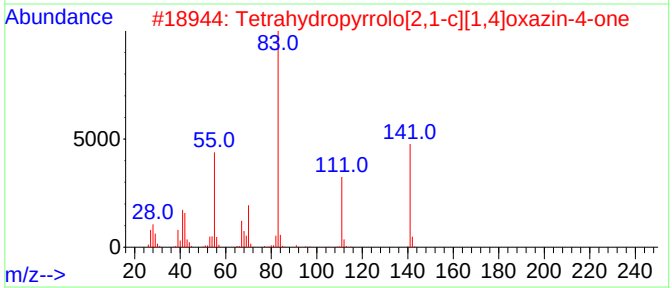


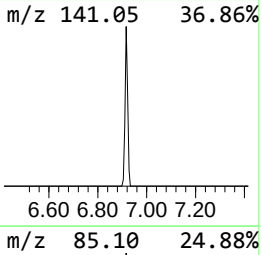


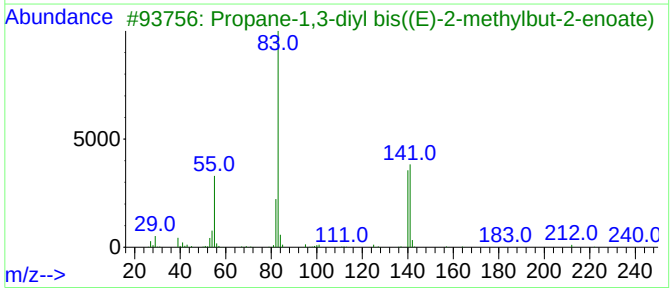


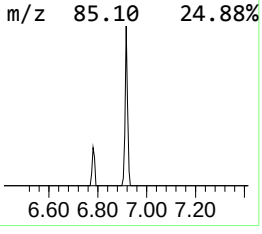












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

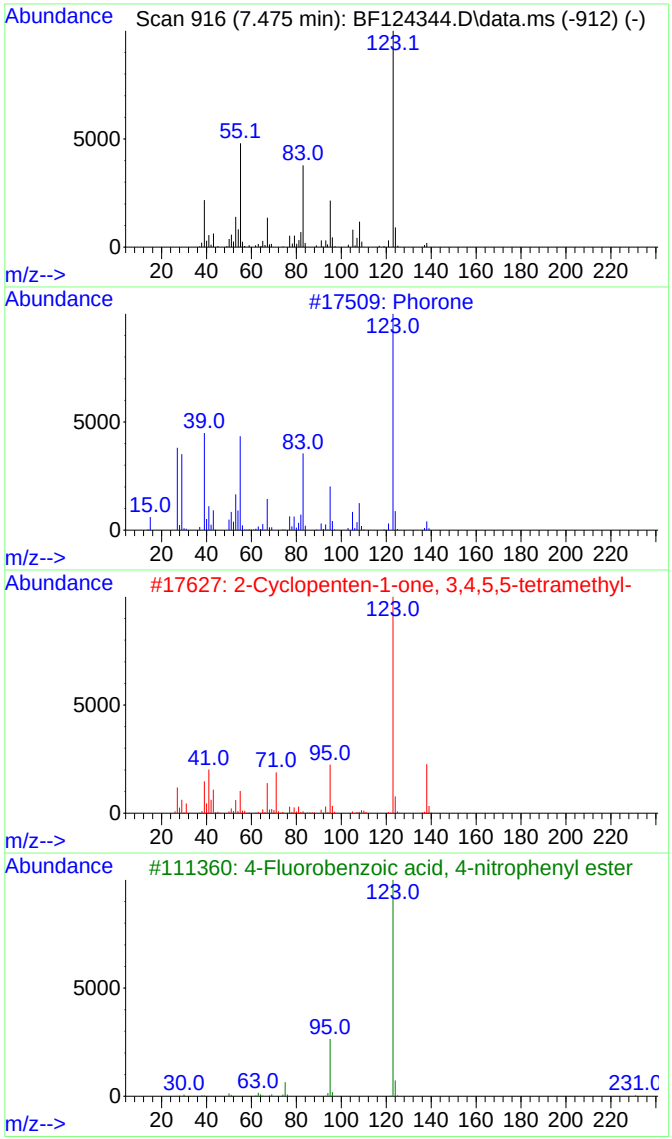
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

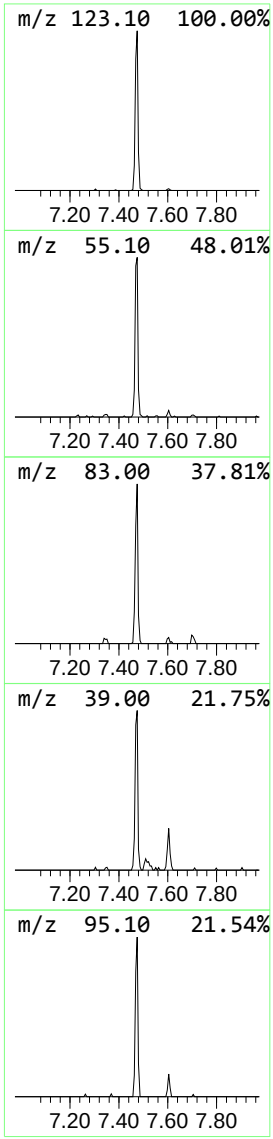
****

Peak Number 5 Phorone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.475	21.75 ng	321433	Naphthalene-d8	8.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phorone	138	C9H14O	000504-20-1	91
2	2-Cyclopenten-1-one, 3,4,5,5-tet...	138	C9H14O	090611-02-2	53
3	4-Fluorobenzoic acid, 4-nitrophe...	261	C13H8FNO4	1000307-45-1	47
4	1,4-Benzenediol, mono-tetradecyl...	306	C20H34O2	013224-40-3	47
5	3-Pyridinol, 2,6-dimethyl-	123	C7H9NO	001122-43-6	47





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
1,3-Dioxolane, ...	2.751	9.3	ng	103839	1	6.781	223508	20.0
4-Penten-2-one,...	3.387	23.5	ng	262540	1	6.781	223508	20.0
3-Penten-2-one,...	4.398	840.1	ng	9388710	1	6.781	223508	20.0
unknown6.916	6.916	12.3	ng	137621	1	6.781	223508	20.0
Phorone	7.475	21.8	ng	321433	2	8.069	295608	20.0