LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016280.D
Acq On : 09 Aug 2018 14:14
Operator : SJ/JU
Sample : J4356-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-32

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_M\METHODS\8270-BM072318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.187	317	323	333	rBV	57012	90538	2.85%	0.565%
2	5.669	399	405	421	rBV	469302	760878	23.97%	4.746%
3	7.310	678	684	697	rBV	274364	483633	15.24%	3.017%
4	7.663	737	744	755	rBV	999677	1569802	49.46%	9.792%
5	8.134	818	824	830	rBV	185439	304718	9.60%	1.901%
6	8.451	871	878	891	rVB	911297	1476349	46.51%	9.209%
7	9.322	1018	1026	1040	rBV	682219	1132786	35.69%	7.066%
8	9.763	1096	1101	1109	rBV2	25269	43005	1.35%	0.268%
9	10.945	1296	1302	1312	rVB	205216	354200	11.16%	2.210%
10	11.457	1383	1389	1395	rBV3	22654	39840	1.26%	0.249%
11	11.516	1395	1399	1410	rVB2	30710	52339	1.65%	0.326%
12	13.386	1711	1717	1724	rBV	1567519	2230715	70.28%	13.915%
13	14.221	1854	1859	1863	rVB	32241	43250	1.36%	0.270%
14	14.768	1946	1952	1959	rVB2	272541	433386	13.65%	2.703%
15	14.827	1959	1962	1967	rBV	25642	41915	1.32%	0.261%
16	15.168	2017	2020	2027	rVB4	22649	32623	1.03%	0.204%
17	16.257	2199	2205	2217	rBV	1359205	1932646	60.89%	12.056%
18	16.421	2230	2233	2241	rVB5	29716	41933	1.32%	0.262%
19	17.504	2412	2417	2424	rBV	318930	459381	14.47%	2.866%
20	18.356	2558	2562	2572	rBV2	72796	126313	3.98%	0.788%
21	18.574	2595	2599	2605	rBV	36885	61918	1.95%	0.386%
22	19.615	2773	2776	2780	rBV5	33001	42028	1.32%	0.262%
23	20.086	2850	2856	2861	rBV	2705144	3173988	100.00%	19.799%
24	21.633	3115	3119	3124	rVB	424901	512022	16.13%	3.194%
25	23.974	3511	3517	3529	rVB2	293552	590570	18.61%	3.684%

Sum of corrected areas: 16030776

LSC Report - Integrated Chromatogram

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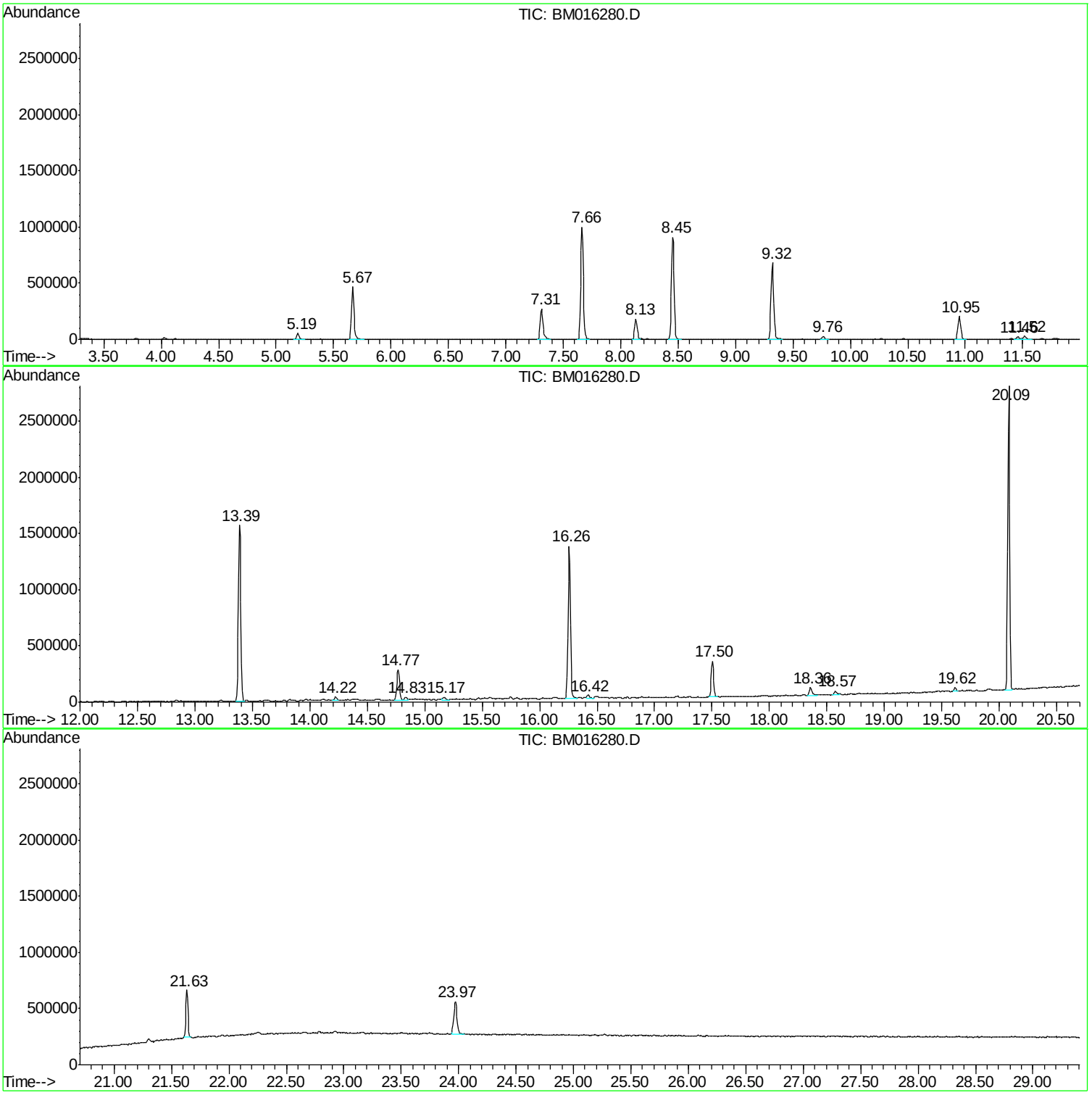
Sample : J4356-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-32

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

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Data File : BM016280.D
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Operator : SJ/JU
Sample : J4356-04
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TIC Integration Parameters: LSCINT.P

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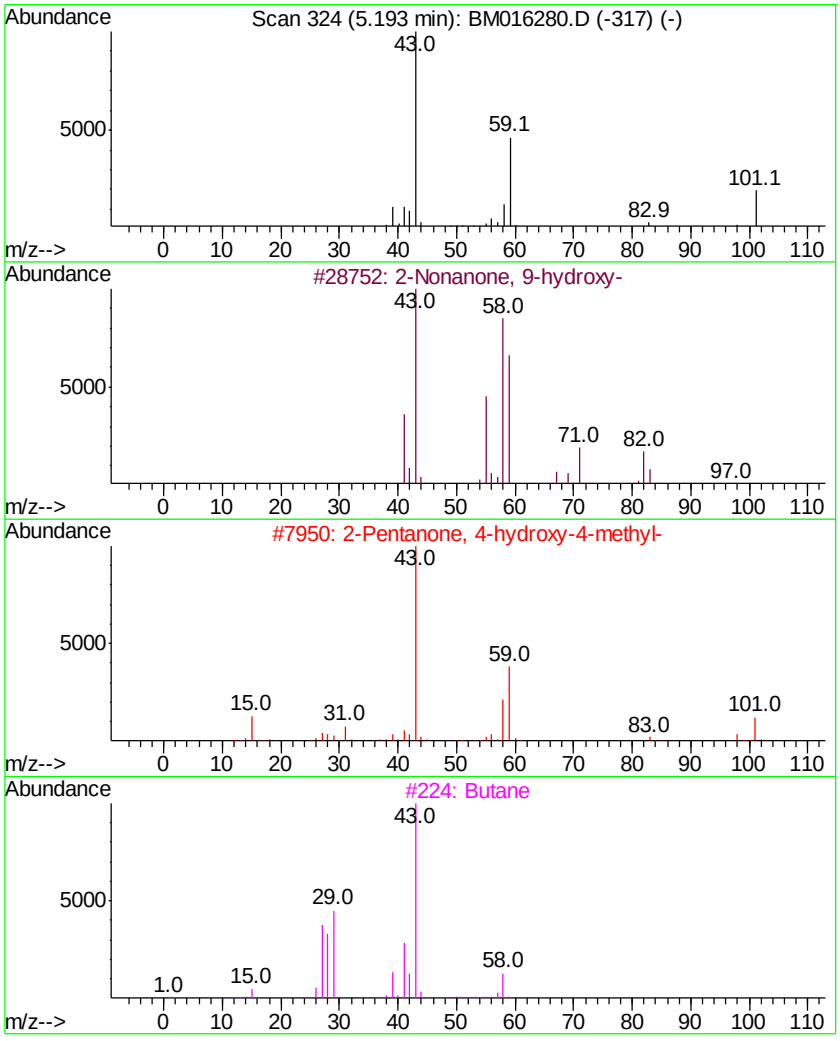
Peak Number 1 unknown5.19 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	5.94 ng	90538	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	39
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
3	Butane	58	C4H10	000106-97-8	16
4	Diacetamide	101	C4H7NO2	000625-77-4	9
5	Propylamine	59	C3H9N	000107-10-8	9



m/z 43.00 100.00%

m/z 59.10 46.40%

m/z 101.10 19.48%

m/z 58.10 12.48%

m/z 39.00 11.48%

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Sample : J4356-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-32

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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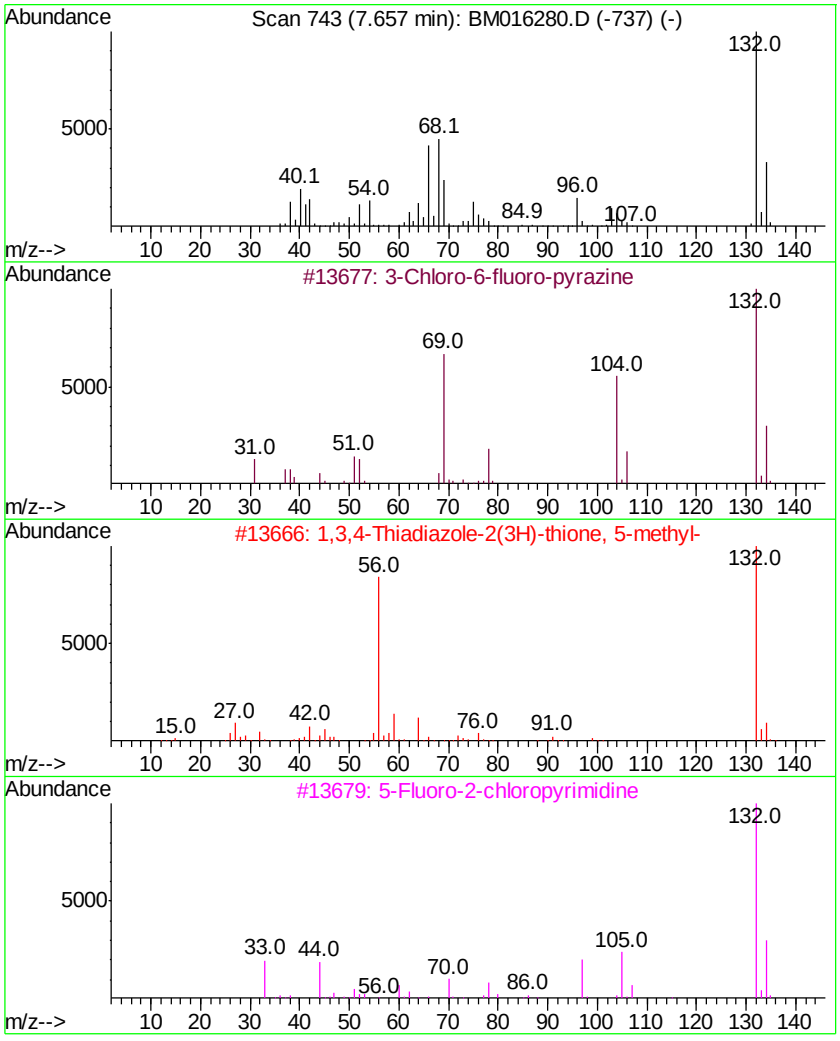
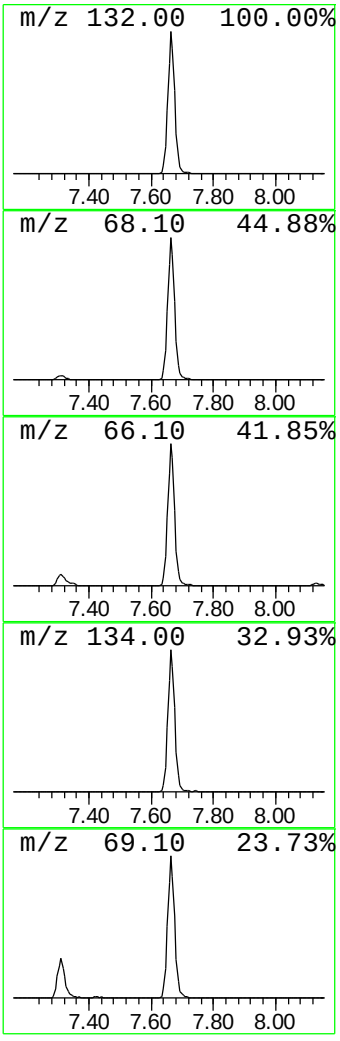
Peak Number 2 unknown7.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	103.03 ng	1569800	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
4	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	14
5	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016280.D
Acq On : 09 Aug 2018 14:14
Operator : SJ/JU
Sample : J4356-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-32

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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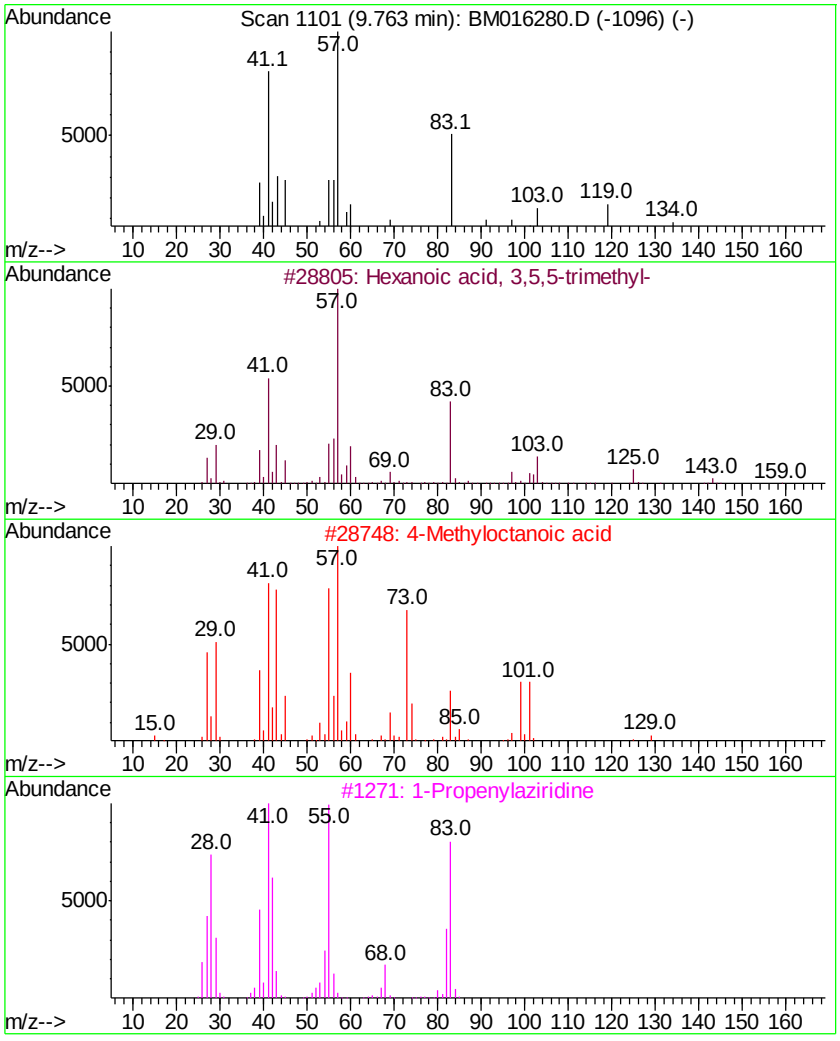
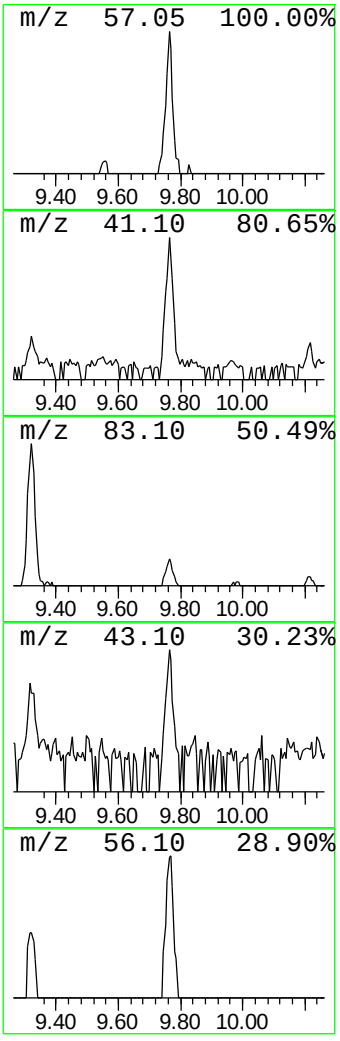
Peak Number 4 Hexanoic acid, 3,5,5-trimet... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.76	2.43 ng	43005	Naphthalene-d8	10.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	64
2	4-Methyloctanoic acid	158	C9H18O2	054947-74-9	33
3	1-Propenylaziridine	83	C5H9N	1000192-51-0	9
4	Propanoic acid, 2,2-dimethyl-, h...	186	C11H22O2	005434-57-1	9
5	1-Hexadecene	224	C16H32	000629-73-2	9





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Data File : BM016280.D
Acq On : 09 Aug 2018 14:14
Operator : SJ/JU
Sample : J4356-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-32

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

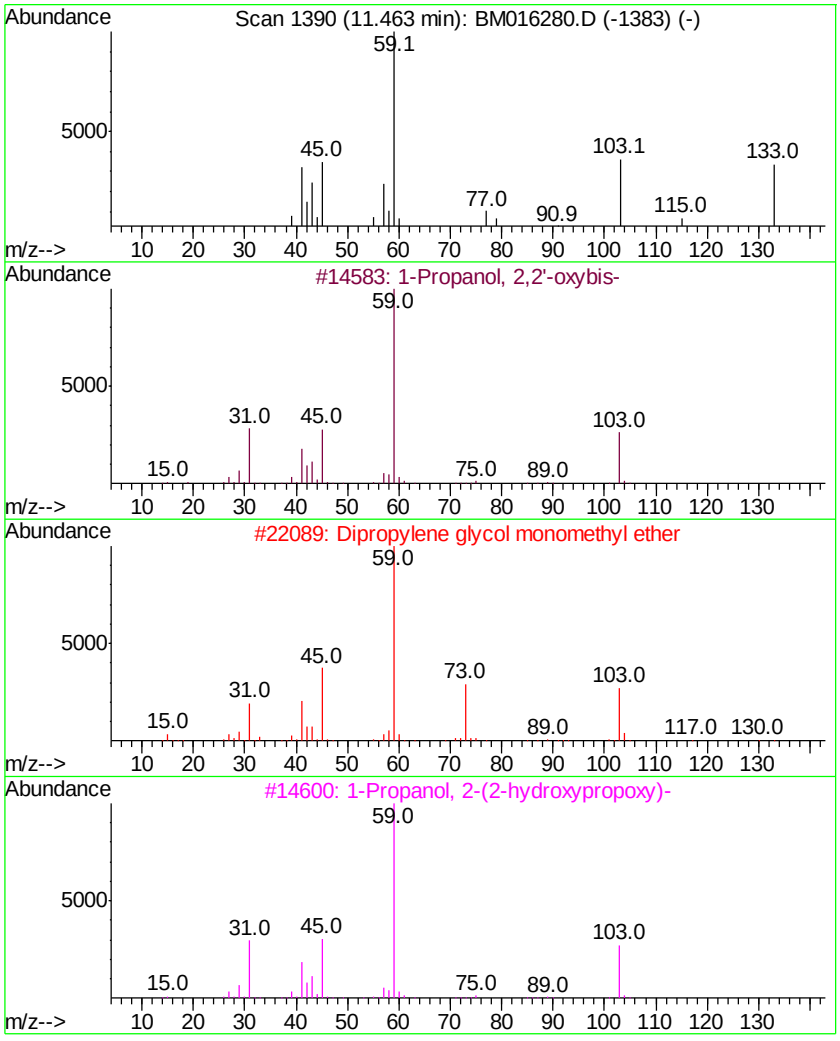
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

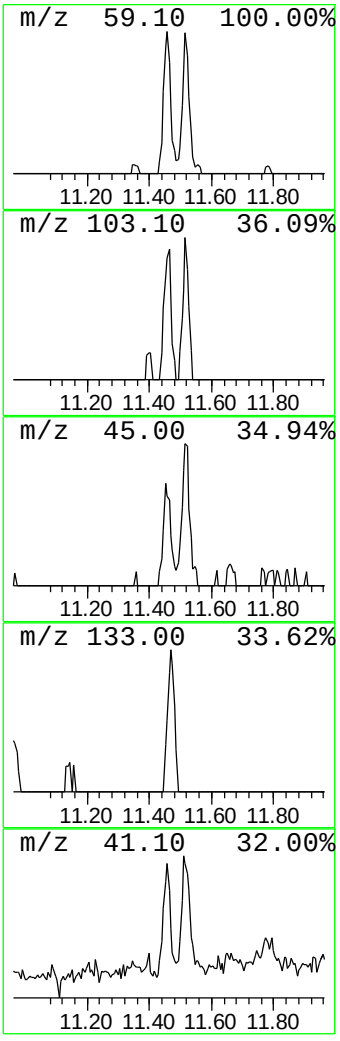
****

Peak Number 5 unknown11.46 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.46	2.25 ng	39840	Naphthalene-d8	10.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	39
2	Dipropylene glycol monomethyl ether	148	C7H16O3	034590-94-8	39
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	39
4	Dipropylene glycol	134	C6H14O3	025265-71-8	38
5	Hexylene Glycol	118	C6H14O2	000107-41-5	33





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Data File : BM016280.D
Acq On : 09 Aug 2018 14:14
Operator : SJ/JU
Sample : J4356-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-32

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

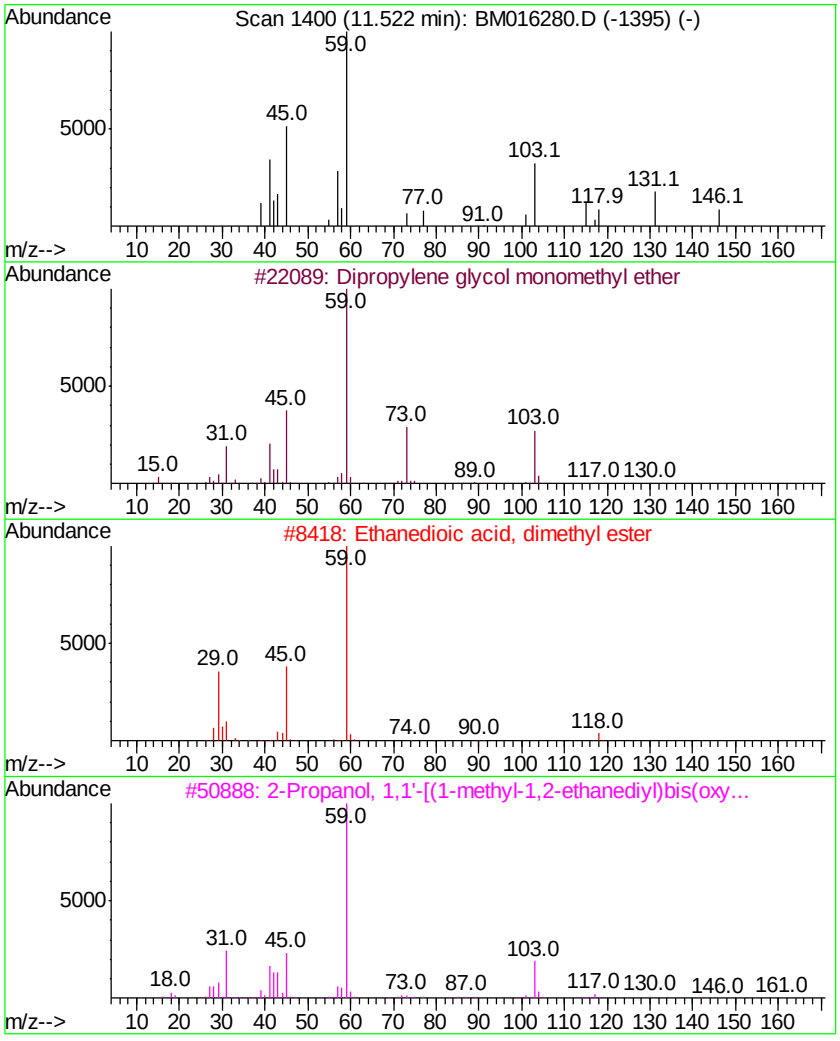
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

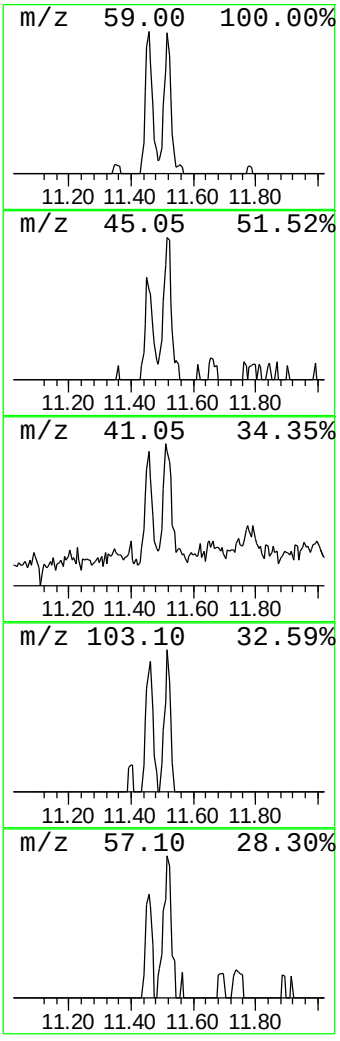
****

Peak Number 6 unknown11.52 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.52	2.96 ng	52339	Naphthalene-d8	10.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dipropylene glycol monomethyl ether	148	C7H16O3	034590-94-8	42
2	Ethanedioic acid, dimethyl ester	118	C4H6O4	000553-90-2	40
3	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	10
4	Butanamide, 3,3-dimethyl-	115	C6H13NO	000926-04-5	9
5	Pentane, 1-ethoxy-	116	C7H16O	017952-11-3	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
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Sample : J4356-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-32

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

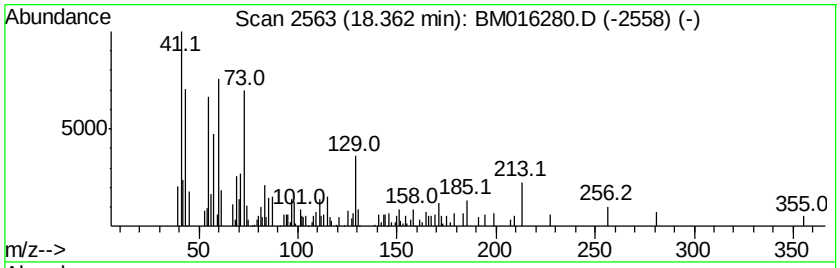
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

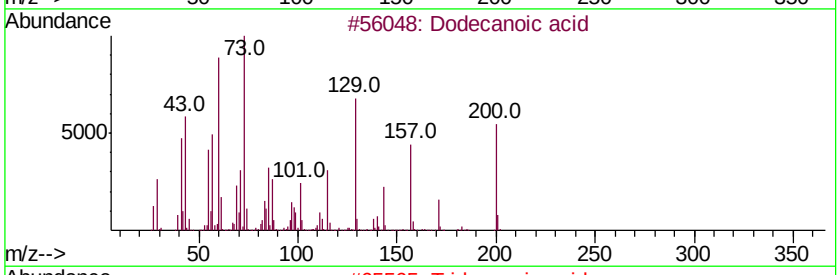
****

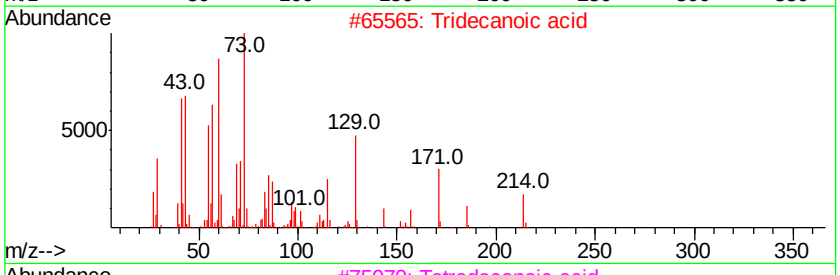
Peak Number 7 Dodecanoic acid Concentration Rank 4

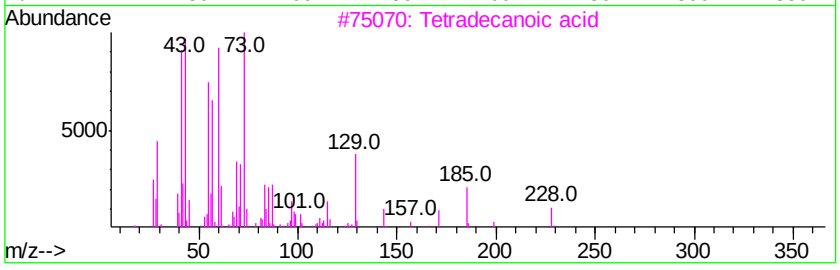
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	5.50 ng	126313	Phenanthrene-d10	17.50

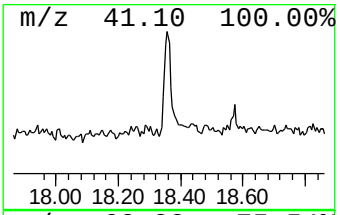
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	72
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4	n-Decanoic acid	172	C10H20O2	000334-48-5	55
5	Undecanoic acid	186	C11H22O2	000112-37-8	47

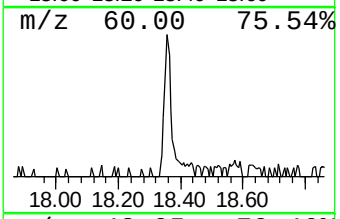


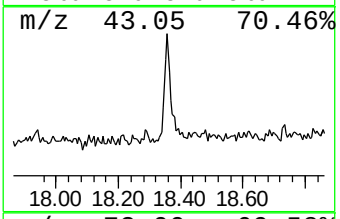


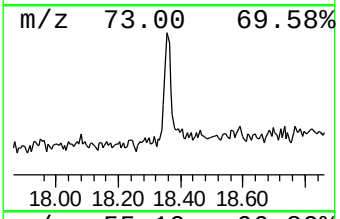


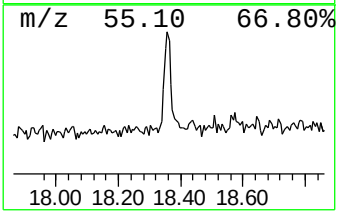












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

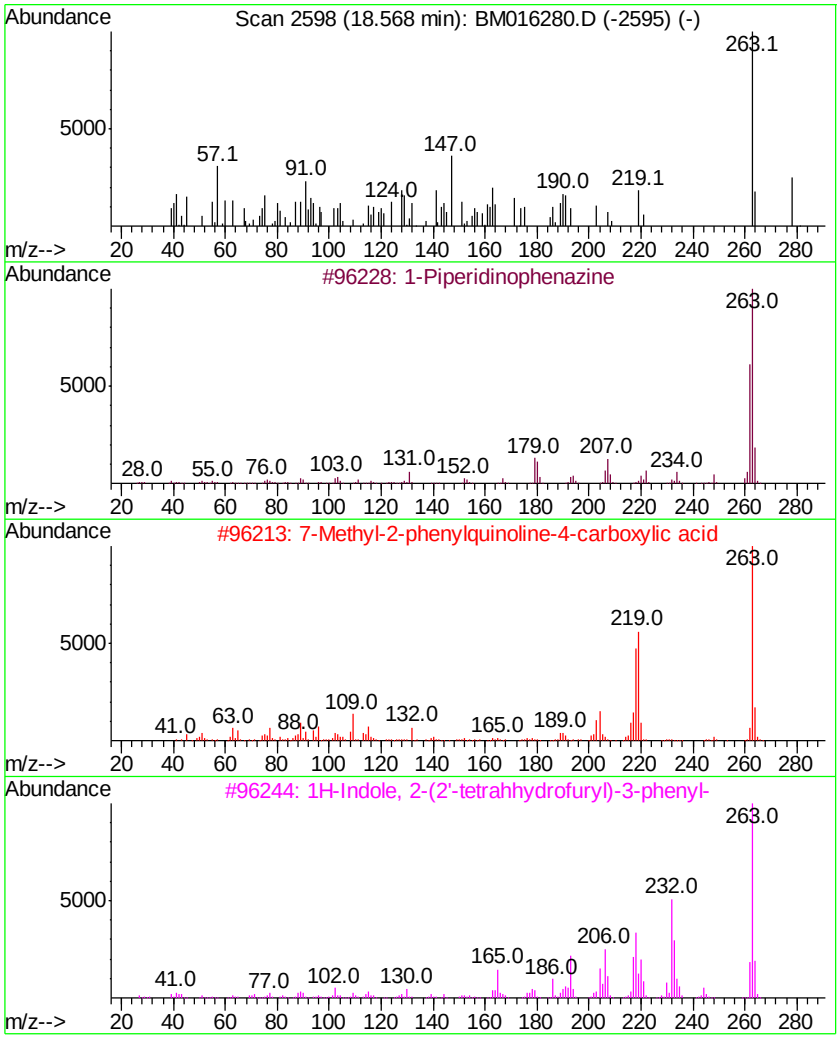
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

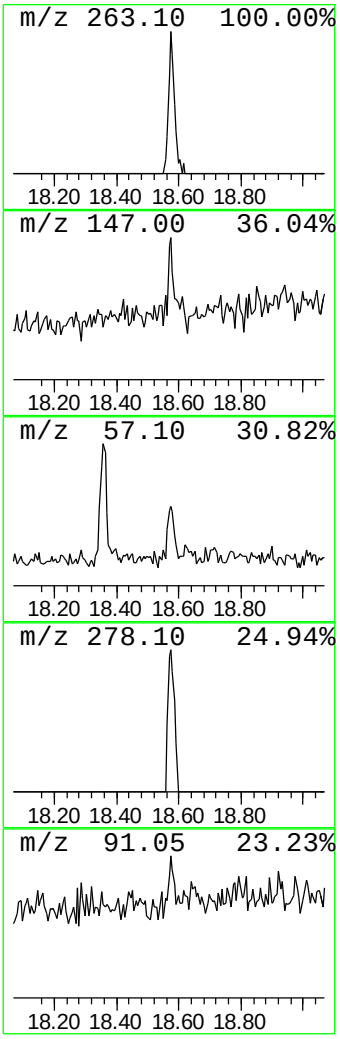
****

Peak Number 8 unknown18.27 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.57	2.70 ng	61918	Phenanthrene-d10	17.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Piperidinophenazine	263	C17H17N3	021942-93-8	47
2	7-Methyl-2-phenylquinoline-4-car...	263	C17H13NO2	181048-54-4	47
3	1H-Indole, 2-(2'-tetrahhydrofurv...	263	C18H17NO	163064-85-5	40
4	Quinoline-4-carboxylic acid, 2-(...	263	C17H13NO2	020389-05-3	38
5	Ethanone, [1-(2,5-diphenyl-2H-1,...	263	C16H13N3O	322647-34-7	37





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown5.19	5.19	5.9	ng	90538	1	8.13	304718	20.0
unknown7.66	7.66	103.0	ng	1569800	1	8.13	304718	20.0
Hexanoic acid, 3,...	9.76	2.4	ng	43005	2	10.95	354200	20.0
unknown11.46	11.46	2.3	ng	39840	2	10.95	354200	20.0
unknown11.52	11.52	3.0	ng	52339	2	10.95	354200	20.0
Dodecanoic acid	18.36	5.5	ng	126313	4	17.50	459381	20.0
unknown18.27	18.57	2.7	ng	61918	4	17.50	459381	20.0