LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM072617\
Data File : BM010973.D
Acq On : 26 Jul 2017 16:38
Operator : SJ/JU
Sample : I4351-25
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 0536

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:\HPCHEM1\BNA_M\METHODS\8270-BM072617.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	3.328	71	75	89	rBV	2142364	2939074	6.55%	0.545%
2	4.587	284	289	298	rVB	386711	532093	1.19%	0.099%
3	5.034	358	365	374	rBV	6673673	8781622	19.57%	1.628%
4	6.598	619	631	645	rBV	6190435	9587855	21.37%	1.778%
5	6.846	666	673	680	rBV	4406847	5916793	13.19%	1.097%
6	6.940	682	689	696	rVB	6216401	9466338	21.10%	1.755%
7	7.287	740	748	759	rVB	7943213	11962042	26.66%	2.218%
8	7.393	759	766	776	rBV	1089057	1675690	3.73%	0.311%
9	7.710	812	820	822	rBV	4845324	7650318	17.05%	1.418%
10	7.740	822	825	835	rVB	5571276	7894221	17.59%	1.464%
11	7.928	848	857	864	rBV	1681253	4144105	9.23%	0.768%
12	8.204	897	904	917	rBV	1908221	3134056	6.98%	0.581%
13	8.451	939	946	953	rVB	3818591	5859648	13.06%	1.086%
14	8.545	953	962	965	rBV	3748886	6551443	14.60%	1.215%
15	8.592	965	970	977	rVB	8251334	12884762	28.71%	2.389%
16	9.104	1048	1057	1067	rBV	5505576	8587079	19.14%	1.592%
17	10.022	1205	1213	1221	rBV	5156383	8233931	18.35%	1.527%
18	10.151	1227	1235	1239	rBV	1361753	2358881	5.26%	0.437%
19	10.204	1239	1244	1254	rVB	6191148	9746853	21.72%	1.807%
20	10.492	1286	1293	1306	rBV	4767090	7346939	16.37%	1.362%
21	12.186	1574	1581	1589	rBV	4083541	6009075	13.39%	1.114%
22	12.663	1654	1662	1673	rVB	10799336	15351057	34.21%	2.846%
23	12.910	1694	1704	1711	rBV	3181742	4757400	10.60%	0.882%
24	13.527	1801	1809	1817	rBV	5412221	7615487	16.97%	1.412%
25	13.775	1841	1851	1859	rBV	13062258	19272115	42.95%	3.573%
26	14.051	1890	1898	1905	rBV2	1998470	2980140	6.64%	0.553%
27	14.445	1956	1965	1972	rBV	11236292	16510833	36.79%	3.061%
28	14.910	2037	2044	2052	rBV	9635234	11696669	26.07%	2.169%
29	15.110	2072	2078	2086	rVB	8952069	12268048	27.34%	2.275%
30	15.339	2110	2117	2127	rBV	14355700	18964416	42.26%	3.516%
31	15.551	2145	2153	2166	rBV	5549101	7619273	16.98%	1.413%
32	16.121	2242	2250	2256	rBV	17258863	22995281	51.24%	4.263%
33	16.810	2358	2367	2376	rVB	2837431	4040638	9.00%	0.749%
34	16.945	2382	2390	2399	rBV	18764945	25553053	56.94%	4.738%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM072617\
Data File : BM010973.D
Acq On : 26 Jul 2017 16:38
Operator : SJ/JU
Sample : I4351-25
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 0536

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:\HPCHEM1\BNA_M\METHODS\8270-BM072617.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	17.810	2531	2537	2542	rVB	15259689	19294731	43.00%	3.577%
36	17.986	2560	2567	2573	rBV	1182340	1503398	3.35%	0.279%
37	19.256	2775	2783	2788	rBV	24350799	33052784	73.66%	6.128%
38	19.474	2813	2820	2831	rBV	21233438	25690511	57.25%	4.763%
39	20.974	3070	3075	3078	rBV	4323584	4623089	10.30%	0.857%
40	21.015	3078	3082	3093	rVB2	17996857	27017856	60.21%	5.009%
41	21.827	3215	3220	3225	rBV	8870452	9863992	21.98%	1.829%
42	22.521	3331	3338	3342	rBV	9936847	16414872	36.58%	3.043%
43	22.574	3342	3347	3356	rVB2	28041018	44874581	100.00%	8.320%
44	23.068	3427	3431	3436	rVB	401207	561529	1.25%	0.104%
45	23.139	3438	3443	3450	rVB	2260712	3866371	8.62%	0.717%
46	23.662	3528	3532	3540	rVB4	407205	722655	1.61%	0.134%
47	24.350	3644	3649	3656	rVB4	405729	775156	1.73%	0.144%
48	25.244	3789	3801	3814	rVB3	12639098	37325309	83.18%	6.920%
49	25.850	3896	3904	3914	rVB	1033145	2889548	6.44%	0.536%

Sum of corrected areas: 539363610

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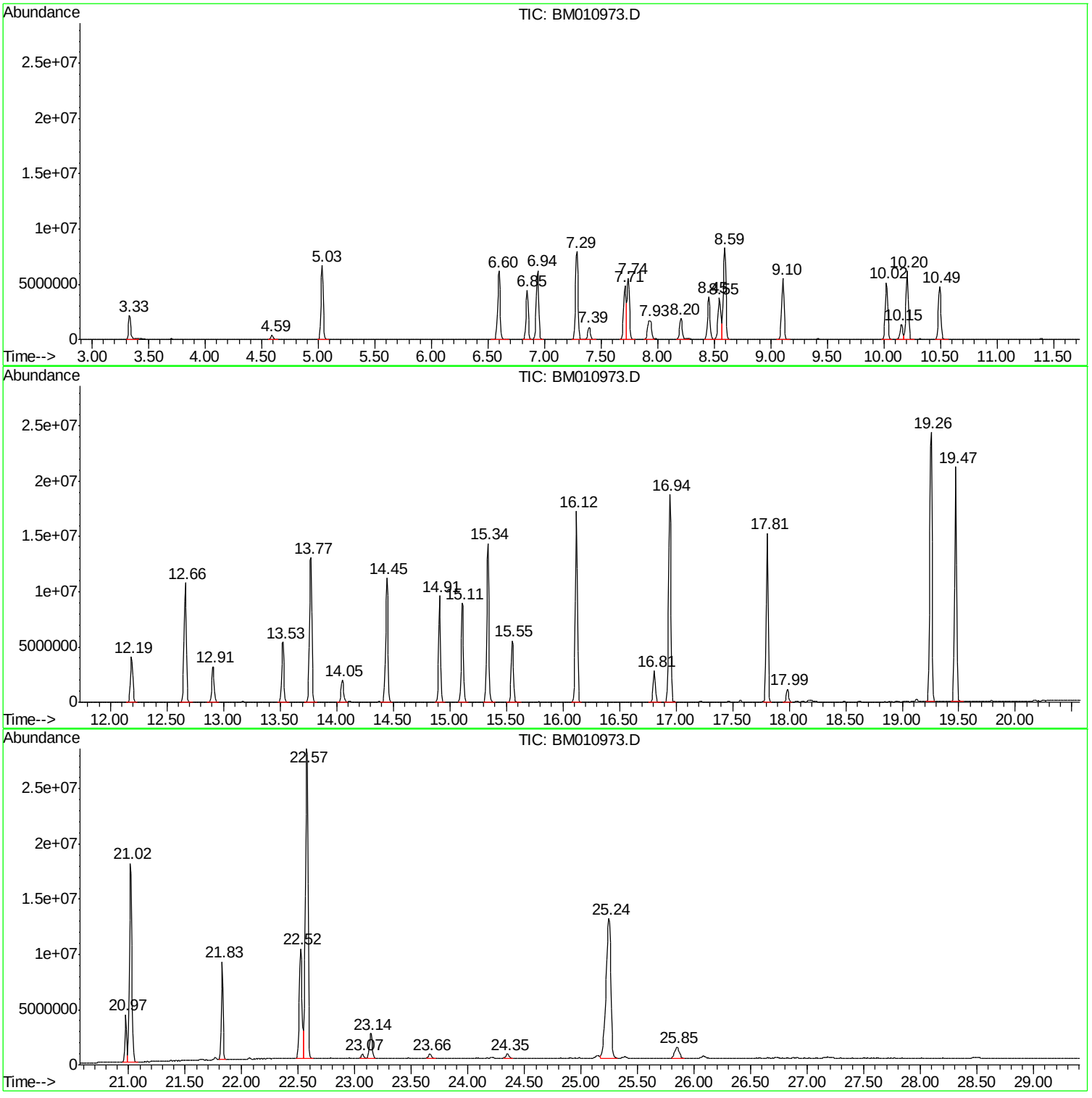
Operator : SJ/JU
Sample : I4351-25
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 0536

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM072617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA M\DATA\BM072617\
Data File : BM010973.D
Acq On : 26 Jul 2017 16:38
Operator : SJ/JU
Sample : I4351-25
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 0536

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM072617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

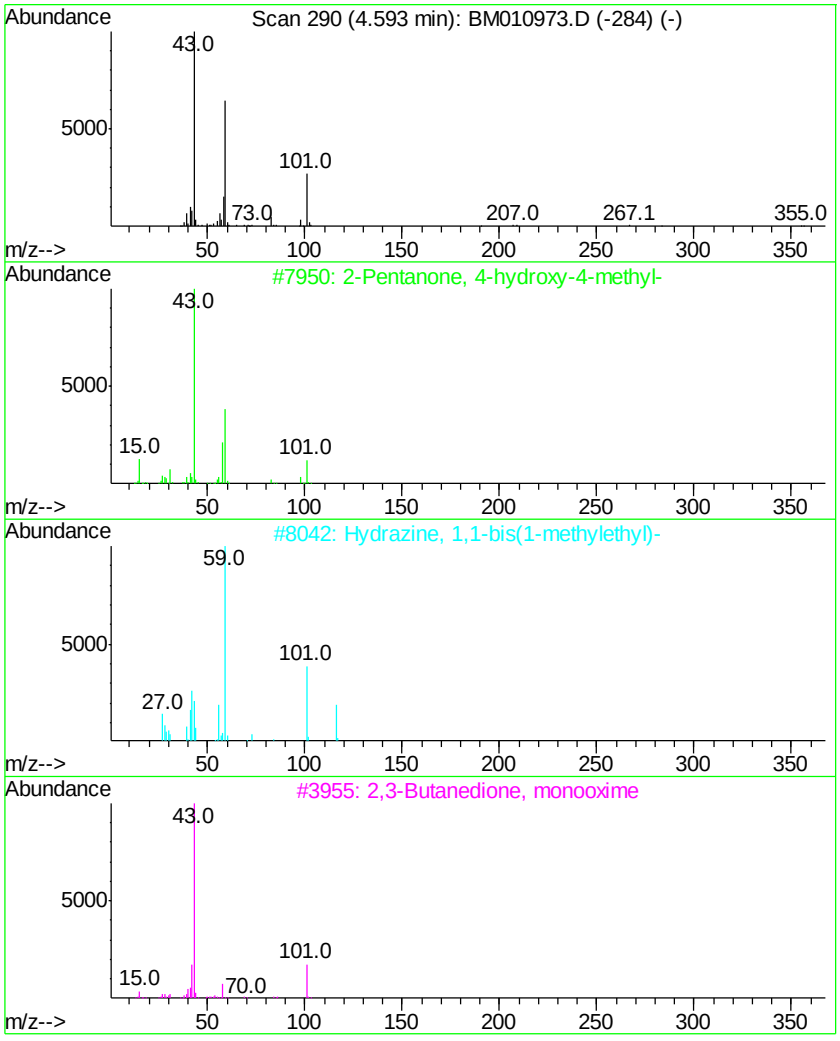
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

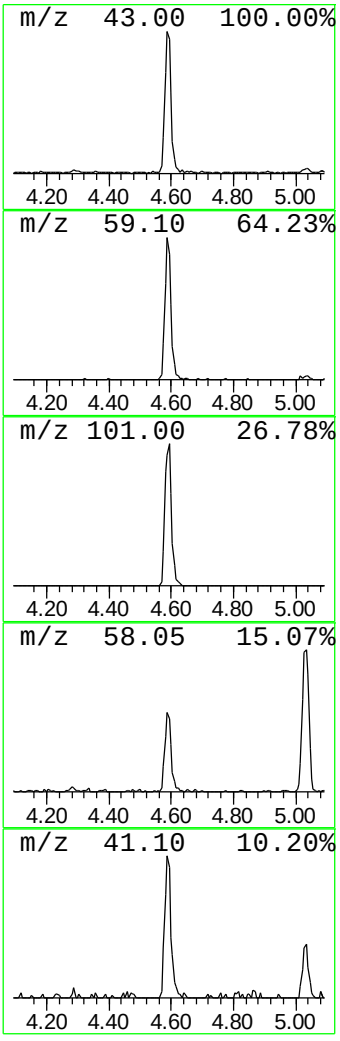
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.59	6.35 ng	532093	1,4-Dichlorobenzene-d4	7.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	47
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	Acetic acid, 10,11-dihydroxy-3,7...	298	C17H30O4	1000194-28-5	25
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	16





Data Path : Z:\HPCHEM1\BNA M\DATA\BM072617\
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Sample : I4351-25
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 0536

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM072617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

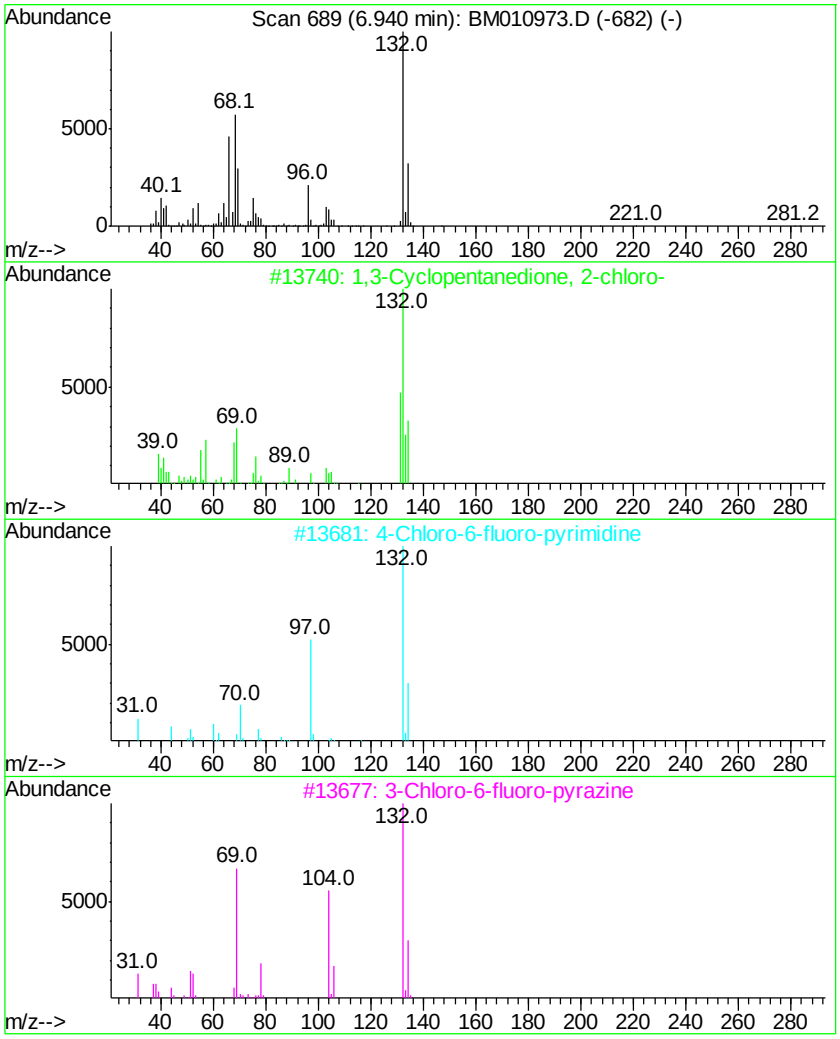
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

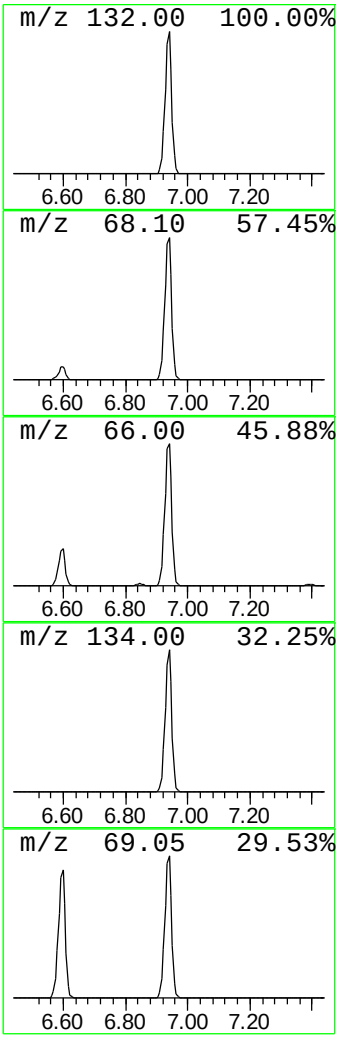
****

Peak Number 2 unknown6.94 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.94	112.98 ng	9466340	1,4-Dichlorobenzene-d4	7.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	16
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10





Data Path : Z:\HPCHEM1\BNA M\DATA\BM072617\
Data File : BM010973.D
Acq On : 26 Jul 2017 16:38
Operator : SJ/JU
Sample : I4351-25
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 0536

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM072617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

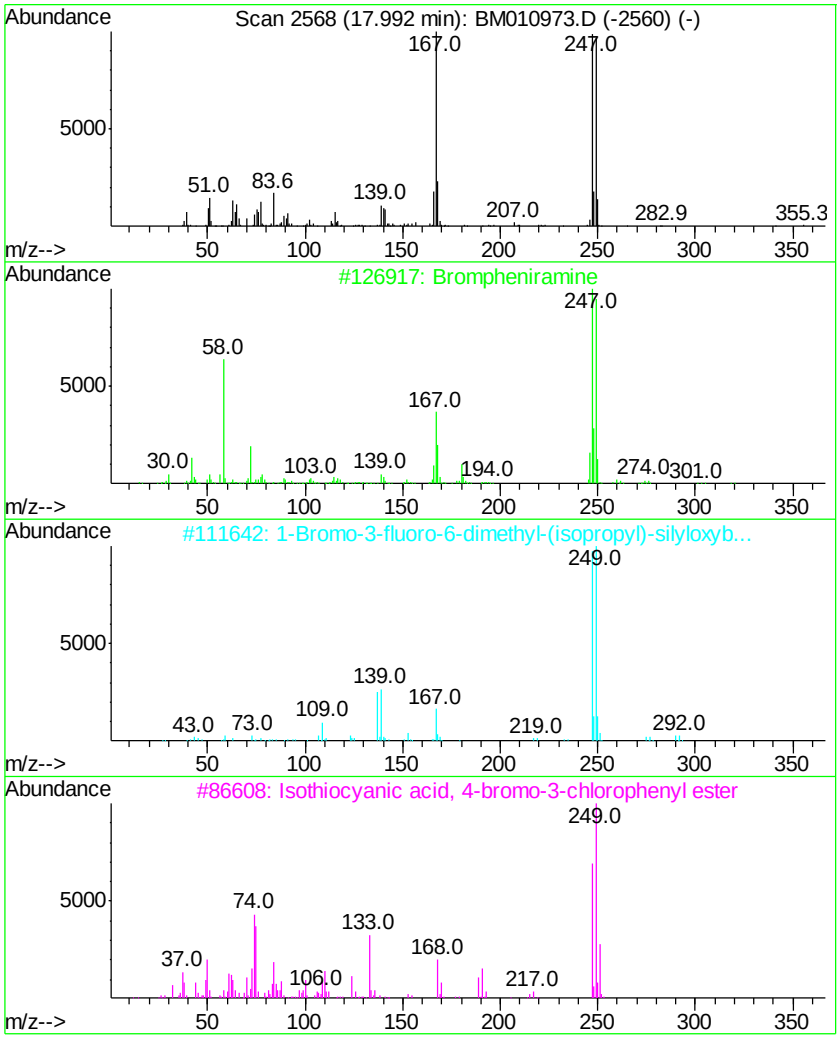
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

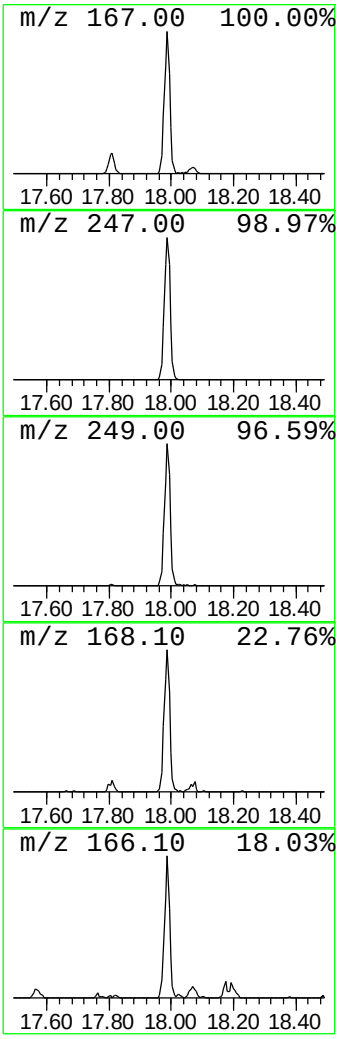
****

Peak Number 3 unknown17.99 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.99	7.44 ng	1503400	Phenanthrene-d10	16.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Brompheniramine	318	C16H19BrN2	000086-22-6	40
2	1-Bromo-3-fluoro-6-dimethyl-(iso...	290	C11H16BrFOSi	1000292-67-3	38
3	Isothiocyanic acid, 4-bromo-3-ch...	247	C7H3BrClNS	032118-33-5	37
4	5H-Indeno[1,2-b]pyridine	167	C12H9N	000244-99-5	25
5	Carbazole	167	C12H9N	000086-74-8	22





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM072617\
Data File : BM010973.D
Acq On : 26 Jul 2017 16:38
Operator : SJ/JU
Sample : I4351-25
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 0536

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM072617.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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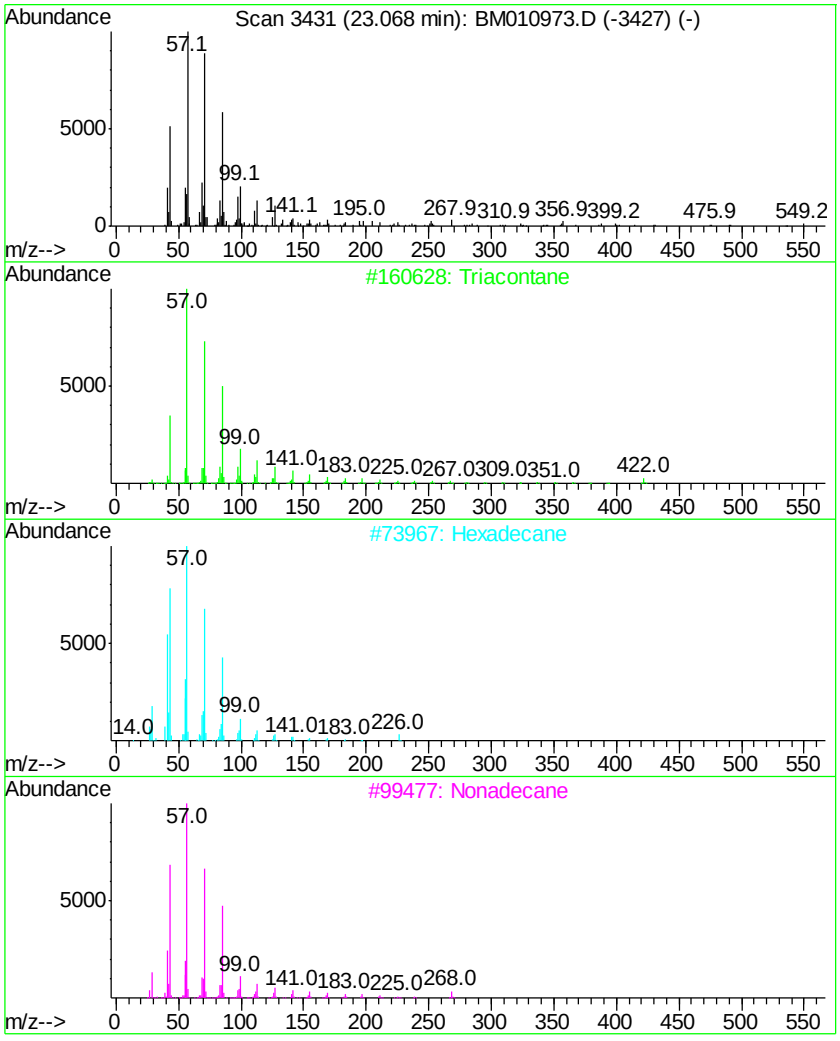
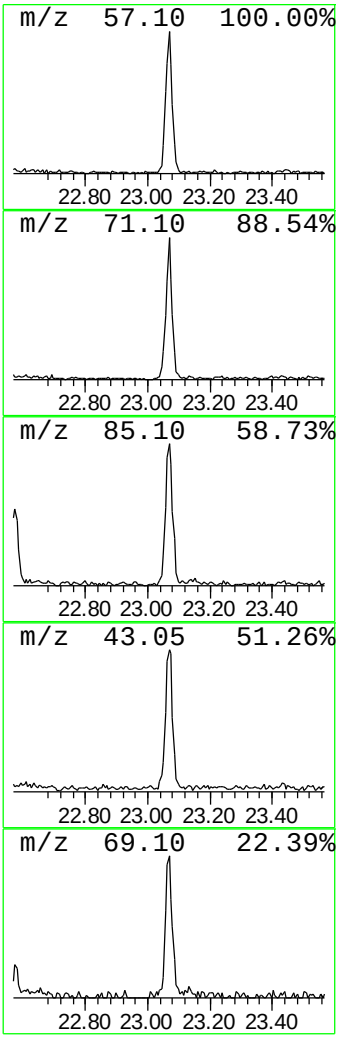
Peak Number 4 Triacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.07	2.90 ng	561529	Perylene-d12	23.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	Hexadecane	226	C16H34	000544-76-3	87
3	Nonadecane	268	C19H40	000629-92-5	87
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	86
5	10-Methylnonadecane	282	C20H42	056862-62-5	86





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Instrument : BNA_M
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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM072617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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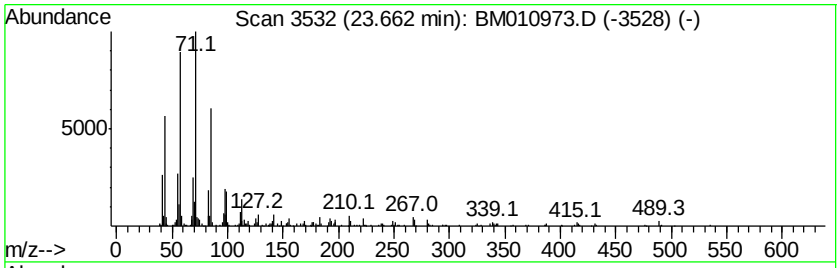
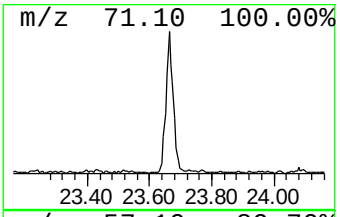
****

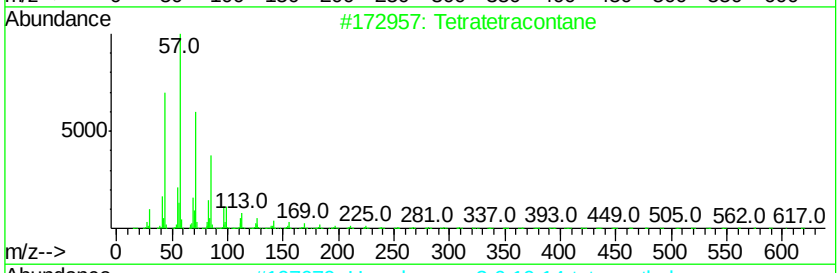
Peak Number 5 Tetratetracontane Concentration Rank 5

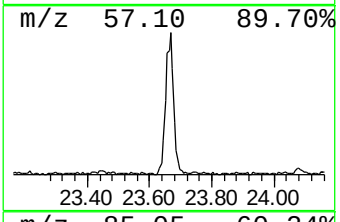
R.T.	EstConc	Area	Relative to ISTD	R.T.
23.66	3.74 ng	722655	Perylene-d12	23.14

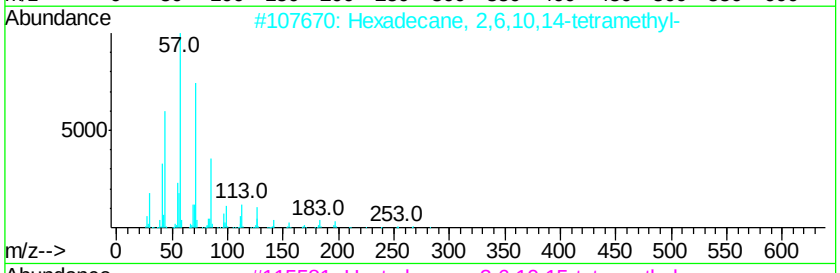
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	83
2	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	76
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	76
4	Octacosane	394	C28H58	000630-02-4	72
5	Nonadecane	268	C19H40	000629-92-5	68

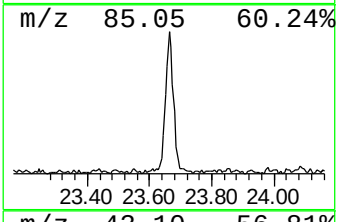


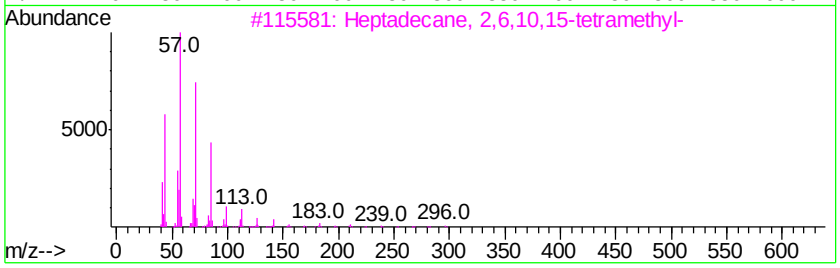


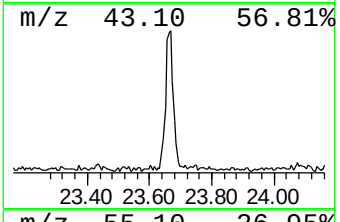


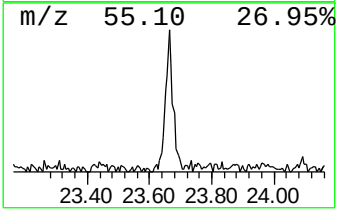












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Instrument : BNA_M
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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM072617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

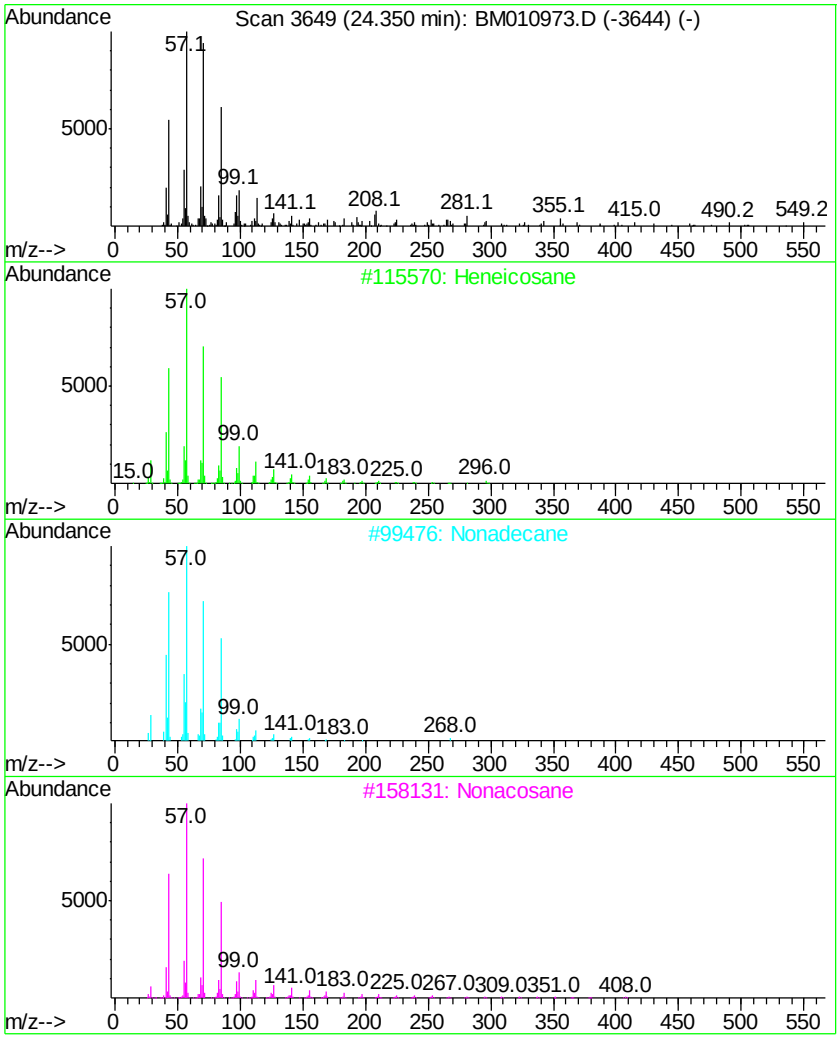
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

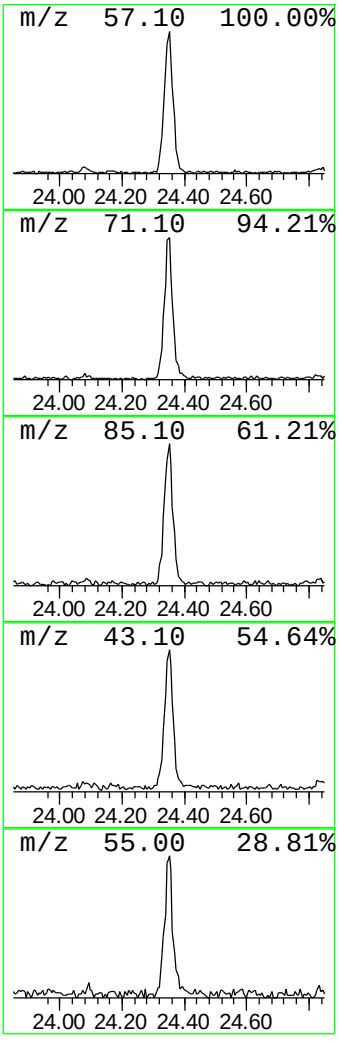
****

Peak Number 6 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.35	4.01 ng	775156	Perylene-d12	23.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Nonadecane	268	C19H40	000629-92-5	87
3	Nonacosane	408	C29H60	000630-03-5	87
4	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	83
5	Heptacosane	380	C27H56	000593-49-7	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM072617\
Data File : BM010973.D
Acq On : 26 Jul 2017 16:38
Operator : SJ/JU
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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 0536

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM072617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.59	6.3	ng	532093	1	7.39	1675690	20.0
unknown6.94	6.94	113.0	ng	9466340	1	7.39	1675690	20.0
unknown17.99	17.99	7.4	ng	1503400	4	16.81	4040640	20.0
Triacontane	23.07	2.9	ng	561529	6	23.14	3866370	20.0
Tetratetracontane	23.66	3.7	ng	722655	6	23.14	3866370	20.0
Heneicosane	24.35	4.0	ng	775156	6	23.14	3866370	20.0